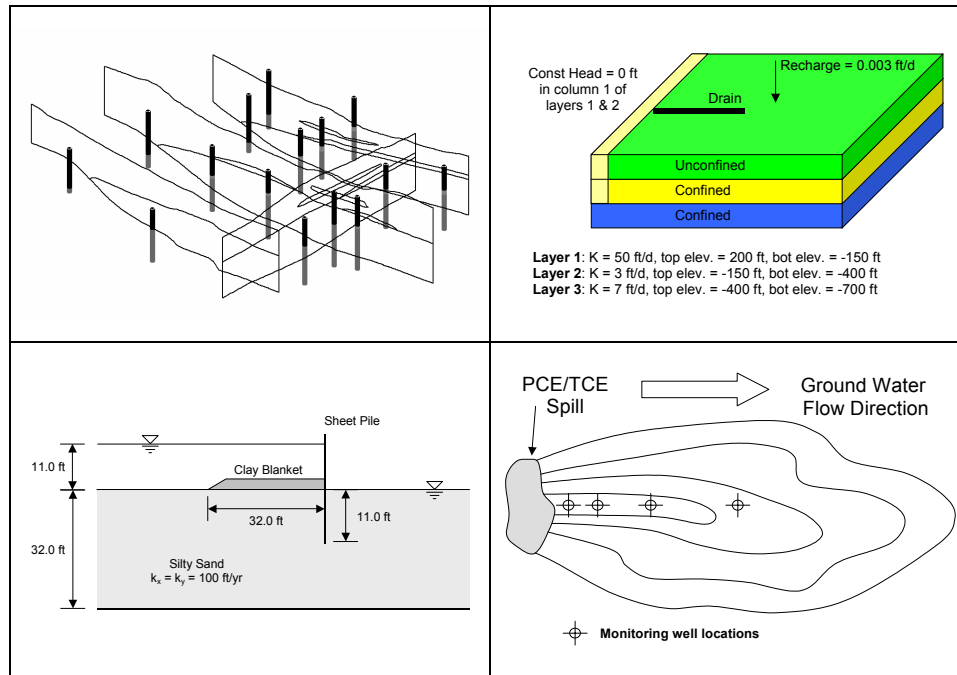


Groundwater Modeling System

TUTORIALS



Volume II

- **MODFLOW, MODPATH, MT3D**
- **Analytic Element Modeling with MODAEM**
- **Calibration**
- **Automated Parameter Estimation**
- **Regional to Local Model Conversion**
- **Transient Data**
- **Stochastic Modeling**

GMS version 5.0

GMS 5.0 Tutorials

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Last Revision: September 7, 2004

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Introduction

This document contains tutorials for the Department of Defense Groundwater Modeling System (GMS). Each tutorial provides training on a specific component of GMS. Since the GMS interface contains a large number of options and commands, you are strongly encouraged to complete the tutorials before attempting to use GMS on a routine basis.

The tutorials are not intended to teach groundwater modeling concepts. They are only meant to illustrate the use of GMS.

In addition to this document, the online GMS Help document also describes the GMS interface. Typically, the most effective approach to learning GMS is to complete the tutorials before browsing the GMS Help document.

1.1 Suggested Order Of Completion

In most cases, the tutorials can be completed in any desired order. However, some of the tutorials are pre-requisites for other tutorials. Tutorials that have other tutorials as pre-requisites will indicate it at the beginning of the tutorial.

1.2 Demo vs. Normal Mode

The interface for GMS is divided into eleven modules. Some of the modules contain interfaces to models such as MODFLOW. Such interfaces are typically contained within a single menu. Since some users may not require all of the

of the modules or model interfaces provided in GMS, modules and model interfaces can be licensed individually. Modules and interfaces that have been licensed are enabled using the *Register* command in the *File* menu. The icons for the unlicensed modules or the menus for model interfaces are dimmed and cannot be accessed.

GMS provides two modes of operation: demo and normal. In normal mode, the modules and interfaces you have licensed are undimmed and fully functional and the items you have not licensed are dimmed and inaccessible. In demo mode, all modules and interfaces are undimmed and functional regardless of which items have been licensed. However, all of the print and save commands are disabled.

The modules and interfaces needed for the tutorial are listed at the beginning of each tutorial. While some of the tutorials may be completed in either normal or demo mode, many of them can only be completed in normal mode. If some of the required items have not been licensed, you will need to obtain an updated password or hardware lock before you complete the tutorial.

1.3 Format

Throughout the tutorials, interface objects like menus or buttons, are shown in italics. Menu commands are given by specifying the menu followed by a “[” symbol followed by the command, like this: “Select the *File | Open* command”. Values that must be entered by the user are given in bold, like this: “Enter **2.0** for the *Hydraulic conductivity*.”

MODFLOW - Grid Approach

Two approaches can be used to construct a MODFLOW simulation in GMS: the grid approach and the conceptual model approach. The grid approach involves working directly with the 3D grid and applying sources/sinks and other model parameters on a cell-by-cell basis. The conceptual model approach involves using the GIS tools in the *Map* module to develop a conceptual model of the site being modeled. The data in the conceptual model are then copied to the grid.

The grid approach to MODFLOW pre-processing is described in this tutorial. In most cases, the conceptual model approach is more efficient than the grid approach. However, the grid approach is useful for simple problems or academic exercises where cell-by-cell editing is necessary. It is not necessary to complete this tutorial before beginning the MODFLOW - *Conceptual Model Approach* tutorial.

2.1 Description of Problem

The problem we will be solving in this tutorial is shown in Figure 2-1. This problem is a modified version of the sample problem described near the end of the MODFLOW *Reference Manual*. Three aquifers will be simulated using three layers in the computational grid. The grid covers a square region measuring 75000 ft by 75000 ft. The grid will consist of 15 rows and 15 columns, each cell measuring 5000 ft by 5000 ft in plan view. For simplicity, the elevation of the top and bottom of each layer will be flat. The hydraulic conductivity values shown are for the horizontal direction. For the vertical direction, we will use some fraction of the horizontal hydraulic conductivity.

Flow into the system is due to infiltration from precipitation and will be defined as recharge in the input. Flow out of the system is due to buried drain tubes, discharging wells (not shown on the diagram), and a lake which is represented by a constant head boundary on the left. Starting heads will be set equal to zero, and a steady state solution will be computed.

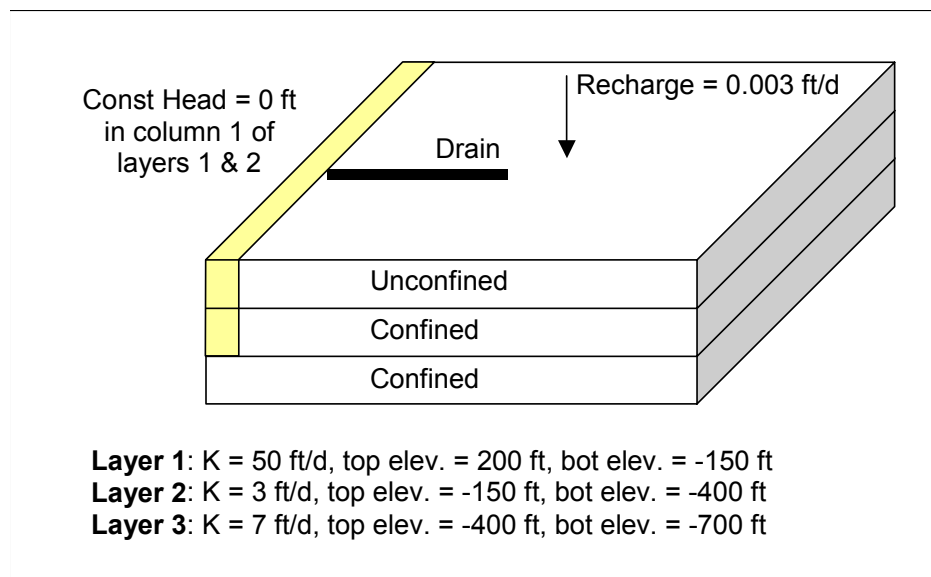


Figure 2-1 Sample Problem to be Solved.

2.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

2.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- MODFLOW

You can see if these components are enabled by selecting the *File | Register* command.

2.4 Units

At this point, we can define the units used in the model. The units we choose will be applied to edit fields in the GMS interface to remind us of the proper units for each parameter.

1. Select the *Edit | Units* command.
2. For *Length*, enter **ft** (for feet). For *Time*, enter **d** (for days). We will ignore the other units (they are not used for flow simulations).
3. Select the *OK* button.

2.5 Creating the Grid

The first step in solving the problem is to create the 3D finite difference grid.

1. Switch to the *3D Grid* module .
2. Select the *Grid | Create Grid* command.
3. Select the section entitled *X-dimension*, enter **75000** for the *Length* value, and **15** for the *Number cells* value.
4. In the section entitled *Y-dimension*, enter **75000** for the *Length* value, and **15** for the *Number cells* value.
5. In the section entitled *Z-dimension*, enter **15000** for the *Length* value, and **3** for the *Number cells* value.

Later, we will enter the top and bottom elevations for each layer of the grid. Thus, the thickness of the cells in the z directions you enter here will not affect the *MODFLOW* computations. The dimension we have entered was chosen to make the cells appear square when displayed prior to entering the layer elevation data.

6. Select the *OK* button.

The grid should appear in your window in plan view. A simplified representation of the grid should also appear in the *Mini-Grid Plot* in the *Tool Palette*.

2.6 Creating the MODFLOW Simulation

The next step in setting up the model is to initialize the *MODFLOW* simulation.

1. Select the *MODFLOW | New Simulation* command.

2.6.1 The Global Package

The input to *MODFLOW* is subdivided into packages. Some of the packages are optional and some are required. One of the required packages is the Global package. We will begin with this package:

Packages

First, we will select the packages.

1. Select the *Packages* button.

The packages dialog is used to specify which of the packages we will be using to set up the model. The Basic package is always used and, therefore, it cannot be turned off. To select the other packages:

2. Select the *Drain, Well* and *Recharge* packages.
3. In the *Solver* section, select the **Strongly Implicit Procedure** package.
4. Select the *OK* button to exit the *Packages* dialog.

The IBOUND Array

The next step is to set up the IBOUND array. The IBOUND array is used to designate each cell as either active ($IBOUND > 0$), inactive ($IBOUND = 0$), or constant head ($IBOUND < 0$). For our problem, all cells will be active, except for the first two layers in the leftmost column, which will be designated as constant head.

5. Select the *IBOUND* button.

The *IBOUND* dialog displays the values of the IBOUND array in a spreadsheet-like fashion, one layer at a time. The edit field in the upper left corner of the dialog can be used to change the current layer. For our problem, we need all of the values in the array to be greater than zero, except for the left column of the top two layers, which should be less than zero. By default, the values in the array should already be greater than zero. Therefore, all we need to do is change the values for the constant head cells. This can be accomplished by entering a value of -1 for each of the thirty constant head cells. However, there is another way to edit the IBOUND array that is much simpler for this case. This method will be described later in the tutorial. For now we will leave all of the cells active.

6. Select the *OK* button to exit the *IBOUND* dialog.

Starting Heads

The next step is to set up the Starting Heads array.

7. Select the *Starting Heads* button.

The Starting Heads array is used to establish an initial head value when performing a transient simulation. Since we are computing a steady state simulation, the initial head for each cell shouldn't make a difference in the final solution. However, the closer the starting head values are to the final head values, the more quickly MODFLOW will converge to a solution. Furthermore, for certain types of layers, if the starting head values are too low, MODFLOW may interpret the cells as being dry. For the problem we are solving, an initial value of zero everywhere should suffice.

The Starting Heads array is also used to establish the head values associated with constant head cells. For our problem, the constant head values are zero. Since all of the starting head values are already zero by default, we don't need to make any changes.

8. Select the *OK* button to exit the *Starting Heads* dialog.

Top and Bottom Elevations

The next step is to set up the top and bottom elevation arrays.

1. Select the *Top Elevation* button.
2. Make sure the *Layer* is **1**.
3. Select the *Constant → Layer* button.
4. Enter a value of **200** and select the *OK* button.
5. Select the *OK* button to leave the *Top Elevations* dialog.

GMS forces the top of a layer to be at the same location as the bottom of the layer above. Thus, we only need to enter the bottom elevations of all the layers now and the tops of the layers will be set automatically.

1. Select the *Bottom Elevation* button.
2. Make sure the *Layer* is **1**.
3. Select the *Constant → Layer* button.
4. Enter a value of **-150** and select the *OK* button.
5. Change the *Layer* to **2**.

6. Select the *Constant* → *Layer* button.
7. Enter a value of **-400** and select the *OK* button.
8. Change the *Layer* to **3**.
9. Select the *Constant* → *Layer* button.
10. Enter a value of **-700** and select the *OK* button.
11. Select the *OK* button to exit the *Bottom Elevation* dialog.
12. Select the *OK* button to exit the *MODFLOW Global Package* dialog.

2.7 Assigning IBOUND Values Directly to Cells

As mentioned above, the IBOUND values can be entered through the IBOUND Array dialog. In some cases, it is easier to assign values directly to cells. This can be accomplished using the *Cell Properties* command. Before using the command, we must first select the cells in the leftmost column of the top two layers.

2.7.1 Viewing the Left Column

To simplify the selection of the cells, we will change the display so that we are viewing the leftmost layer.

1. Choose the *View the J Axis* button .

The grid appears very thin. To make things easier, we will increase the Z magnification so that the grid appears stretched in the vertical direction.

2. Select the *Display | Settings* command.
3. Change the *Z magnification* to **15**.
4. Select the *OK* button.

2.7.2 Selecting the Cells

To select the cells:

1. Choose the *Select Cells* tool .
2. Change the column to **1** in the *Mini-Grid Display* and hit the TAB key.

Notice that we are now viewing column number one (the leftmost column).

3. Drag a box around all of the cells in the top two layers of the grid.

2.7.3 Changing the IBOUND Value

To edit the IBOUND value:

1. Select the *MODFLOW | Cell Properties* command.
2. Change the *IBOUND* option to **Spec. head**.
3. Select the *OK* button to exit the *Cell Properties* dialog.
4. To unselect the selected cells, click anywhere outside the grid.
5. Select the *View the K Axis* button .

Notice that a symbol is displayed in the cells we edited, indicating that the cells are constant head cells.

2.7.4 Checking the Values

To ensure that the IBOUND values were entered correctly:

1. Select the *MODFLOW | Global Options* command.
2. Select the *IBOUND* button.
3. Choose the up arrow to the right of the layer field in the upper left corner of the dialog to cycle through the layers.

Notice that the leftmost column of cells in the top two layers all have a value of -1. Most of the *MODFLOW* input data can be edited in GMS using either a spreadsheet-like dialog such as this, or by selecting a set of cells and entering a value directly, whichever is most convenient.

4. Select the *OK* button to exit the *IBOUND Array* dialog.
5. Select the *OK* button to exit the *MODFLOW Global Package* dialog.

2.8 The LPF Package

The next step in setting up the model is to enter the data for the Layer Property Flow (LPF) package. The LPF package computes the conductances between each of the grid cells and sets up the finite difference equations for the cell-to-cell flow.

To enter the LPF data:

1. Select the *MODFLOW | LPF Package* command.

2.8.1 Layer Types

The options in the *Layer Data* section of the dialog are used to define the layer type and hydraulic conductivity data for each layer. For our problem, we have three layers. The top layer is unconfined, and the bottom two layers are confined. The default layer type in GMS is “convertible”, which means the layer can be confined or unconfined. Thus, we don’t need to change the layer types.

2.8.2 Layer Parameters

The buttons in the *Layer Data* section of the dialog are for entering the parameters necessary for computing the cell-to-cell conductances. MODFLOW requires a set of parameters for each layer depending on the layer type.

2.8.3 Top Layer

First, we will enter the data for the top layer:

1. Select the *Horizontal Hydraulic Conductivity* button.
2. Select the *Constant → Layer* button.
3. Enter a value of **50**.
4. Select the *OK* button.
5. Select the *OK* button to exit the *Horizontal Hydraulic Conductivity* dialog.
6. Repeat this process to enter a value of **10** for the vertical anisotropy.

2.8.4 Middle Layer

Next, we will enter the data for the middle layer:

1. Select the up arrow to the right of the layer edit field in the *Layer Data* section to switch to layer 2.

Enter the following values for layer 2:

Parameter	Value
Horizontal Hydraulic Conductivity	3 ft/d
Vertical Anisotropy	5

2.8.5 Bottom Layer

Switch to layer 3 and enter the following values:

Parameter	Value
Horizontal Hydraulic Conductivity	7 ft/d
Vertical Anisotropy	5

This completes the data entry for this dialog.

1. Select the *OK* button to exit the *MODFLOW LPF Package* dialog.

2.9 The Recharge Package

Next, we will enter the data for the Recharge package. The Recharge package is used to simulate recharge to an aquifer due to rainfall and infiltration. To enter the recharge data:

1. Select the *MODFLOW | Source/Sink Packages* submenu and the *Recharge Package* command.
2. Select the *Constant* → *Array* button.
3. Enter a value of **0.003** and click *OK*.
4. Select the *OK* button to exit the *Recharge Package* dialog.

2.10 The Drain Package

We will now define the row of drains in the top layer of the model. To define the drains, we must first select the cells where the drains are located, and then select the *Point Sources/Sinks* command.

2.10.1 Selecting the Cells

The drains are located in the top layer (layer 1). Since this is the current layer, we don't need to change the view.

We need to select the cells on columns 2-10 of row 8. To select the cells:

1. Choose the *Select Cells* tool .
2. Select the cell at i=8, j=2.

3. Notice that as you move the cursor across the grid, the *ijk* indices of the cell beneath the cursor are displayed in the *Edit Window* at the bottom of the screen.
4. Hold down the *Shift* key to invoke the multi-select mode and select the cells on columns 3-10 of the same row as the cell you have already selected (Figure 2-2).

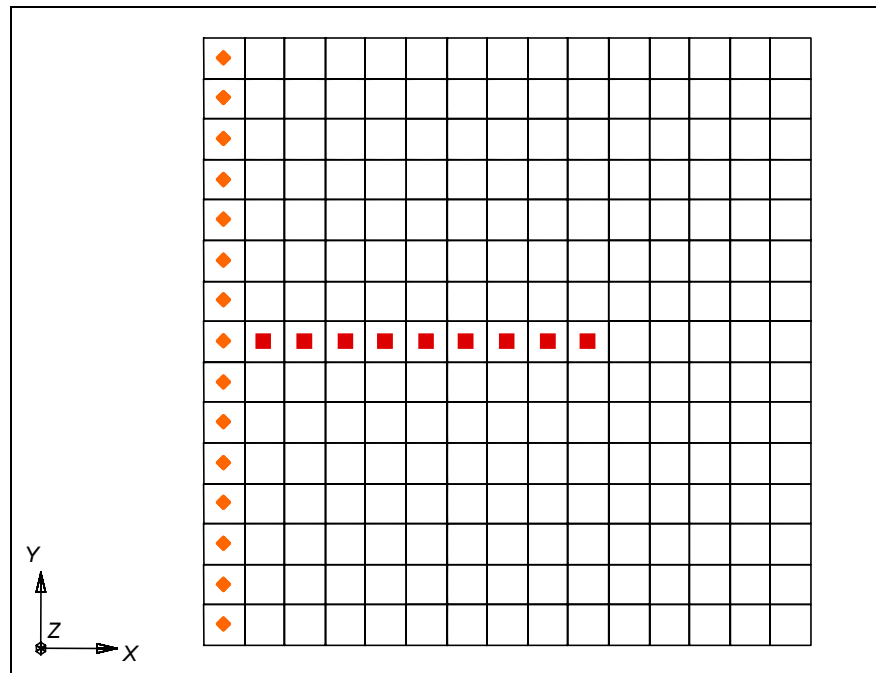


Figure 2-2 Cells to be Selected.

2.10.2 Assigning the Drains

To assign drains to the cells:

1. Select the *MODFLOW | Sources/Sinks* command.
2. Select the *Drain* tab.
3. Select the *New* button. This adds a new instance of a drain to each of the selected cells.

At this point we must enter an elevation and a conductance for the selected drains. The drains all have the same conductance but the elevations are not all the same.

1. Enter the following values for the elevations and conductances of the drains:

ID	Elevation	Conductance
107	0	80,000
108	0	80,000
109	10	80,000
110	20	80,000
111	30	80,000
112	50	80,000
113	70	80,000
114	90	80,000
115	100	80,000

2. Select the *OK* button.
3. Unselect the cells by clicking anywhere outside the grid.

2.11 The Well Package

Next, we will define several wells by selecting the cells where the wells are located and using the *Point Sources/Sinks* command.

2.11.1 Top Layer Wells

Most of the wells are in the top layer but some are in the middle and bottom layers. We will define the wells in the top layers first.

1. While holding down the *Shift* key, select the cells shown in Figure 2-3.

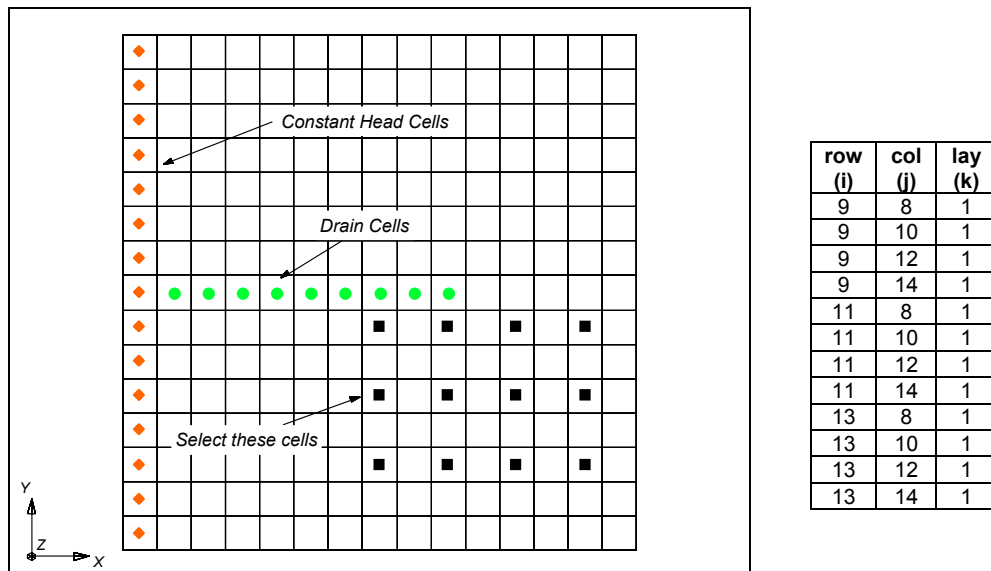


Figure 2-3 Cells to be Selected on Top Layer

2. Select the *MODFLOW | Sources/Sinks* command.
3. Select the *Well* tab.

4. Select the *New* button.
5. Enter a *Flow* value of **-432,000** for all the wells (a negative value signifies extraction).
6. Select the *OK* button.
7. Unselect the cells by clicking anywhere outside the grid.

2.11.2 Middle Layer Wells

Next, we will define some wells on the middle layer. First, we need to view the middle layer.

1. Select the *Decrement* button ↓ in the *Mini-Grid Plot*.

To select the cells:

2. While holding down the *Shift* key, select the cells are shown in Figure 2-4.

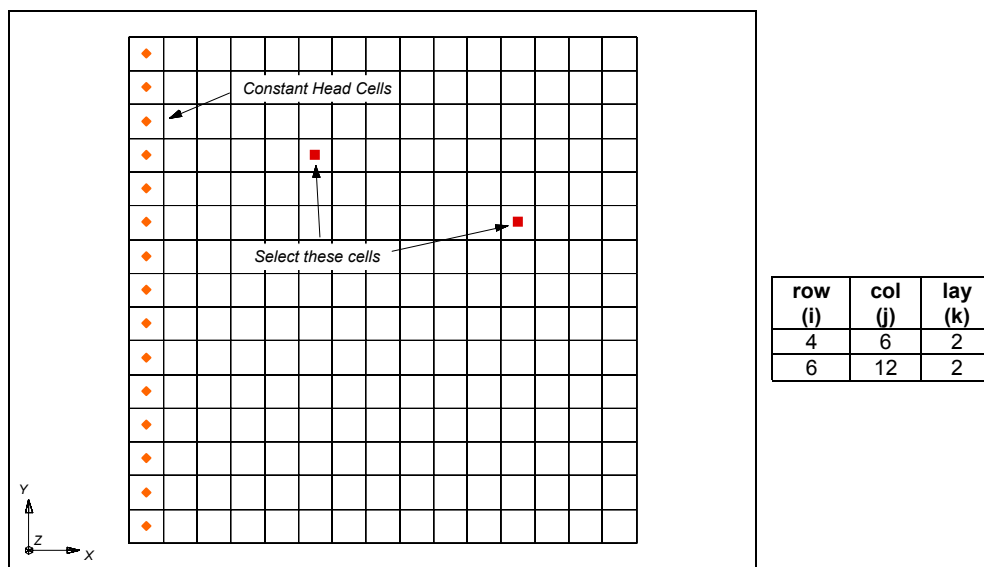


Figure 2-4 Cells to be Selected on Middle Layer.

3. Select the *MODFLOW | Sources/Sinks* command.
4. Select the *Well* tab.
5. Select the *New* button.
6. Enter a *Flow* value of **-432,000** for both wells.

7. Select the *OK* button.
8. Unselect the cells by clicking anywhere outside the grid.

2.11.3 Bottom Layer Well

Finally, we will define a single well on the bottom layer. To view the bottom layer:

1. Select the *Decrement* button ↓ in the *Mini-Grid Plot*.
2. Select the cell is shown in Figure 2-5.

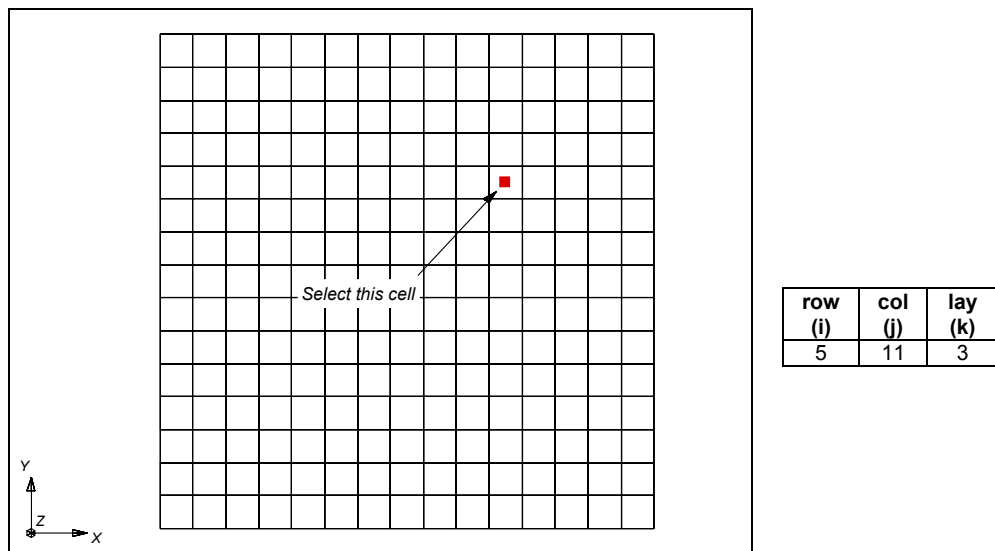


Figure 2-5 Cell to be Selected on Bottom Layer.

3. Select the *MODFLOW | Sources/Sinks* command.
4. Select the *Well* tab.
5. Select the *New* button.
6. Enter a *Flow* value of **-5**.
7. Select the *OK* button.
1. Unselect the cells by clicking anywhere outside the grid.

Now that all of the wells have been defined, we can go back to the top layer.

2. Select the *Increment* button ↑ twice in the *Mini-Grid Plot*.

2.12 Checking the Simulation

At this point, we have completely defined the MODFLOW data and we are ready to run the simulation. However, before saving the simulation and running MODFLOW, we should run the MODFLOW *Model Checker* and check for errors. Because of the significant amount of data required for a MODFLOW simulation, it is often easy to omit some of the required data or to define inconsistent or incompatible options and parameters. Such errors will either cause MODFLOW to crash or to generate an erroneous solution. The purpose of the *Model Checker* is to analyze the input data currently defined for a MODFLOW simulation and report any obvious errors or potential problems. Running the *Model Checker* successfully does not guarantee that a solution will be correct. It simply serves as an initial check on the input data and can save a considerable amount of time that would otherwise be lost tracking down input errors.

To run the *Model Checker*:

1. Select the *MODFLOW | Check Simulation* command.
2. Select the *Run Check* button.

A list of messages are shown for each of the MODFLOW input packages. If you have done everything correctly, there should be no errors for any of the packages. When there is an error, if you select or highlight the error, when appropriate, GMS selects the cells or layers associated with the problem.

3. Select the *Done* button to exit the *Model Checker*.

2.13 Saving the Simulation

Now we are ready to save the simulation and run MODFLOW.

1. Select the *File | Save As* command.
2. Move to the directory titled **tutfiles\modfgrid**
3. Change the file name to **gridmod.gpr**.
4. Select the *Save* button.

2.14 Running MODFLOW

We are now ready to run MODFLOW:

1. Select the *MODFLOW | Run MODFLOW* command.

At this point MODFLOW is launched in a new window. The super file name is passed to MODFLOW as a command line argument. MODFLOW opens the file and begins the simulation. As the simulation proceeds, you should see some text output in the window reporting the solution progress.

2. When MODFLOW finishes, select the *Close* button.

2.15 Viewing the Solution

GMS reads the solution in automatically when you close the MODFLOW window. At this point you should see a set of head contours for the top layer. You may also see some cells containing a blue triangle symbol. These cells are flooded, meaning the computed water table is above the top of the cell.

2.15.1 Changing Layers

To view the solution on the middle layer:

1. Select the *Decrement* button ↓ in the *Mini-Grid Plot*.

To view the solution on the bottom layer:

2. Select the *Decrement* button ↓.

To return to the top layer:

3. Select the *Increment* button ↑ twice.

2.15.2 Color Fill Contours

You can also display the contours using a color fill option.

1. Select the *Data | Contour Options* command in.
2. Change the *Contour Method* to **Color Fill**.
3. Select the *OK* button.

2.15.3 Color Legend

Next, we will display a color legend.

1. Select the *Data | Color Ramp Options* command.
2. Turn on the *Legend* option.
3. Select the *OK* button.

2.16 Conclusion

This concludes the *MODFLOW - Grid Approach* tutorial. Here are the things that you should have learned in this tutorial:

- You can specify which units you are using and GMS will display the units next to input fields to help you input the appropriate value. GMS does not do any unit conversions for you.
- The MODFLOW menu is in the 3D Grid module.
- The MODFLOW packages you want to use in your model can be selected by choosing the *MODFLOW | Global Options* command and clicking the Packages button.
- Most MODFLOW array data can be edited in two ways: via a spreadsheet, or by selecting grid cells and using the *MODFLOW | Cell Properties* command.
- Wells, Drains etc. can be created and edited by selecting the grid cell(s) and choosing the *MODFLOW | Sources/Sinks* command.
- You can use the *Model Checker* to analyze the input data and check for errors.
- In Ortho mode, only one row, or column, or layer of the 3D grid is visible at a time.

MODAEM is a single-layer, steady-state analytic element groundwater flow model that has been enhanced for use with GMS. This chapter introduces MODAEM to the new user and illustrates the use of GMS for analytic element modeling.

3.1 A Short Introduction to the Analytic Element Method

This section introduces new modelers to the analytic element method (AEM). The AEM allows modelers to rapidly model groundwater flow problems using a conceptual modeling toolkit like GMS. MODAEM and GMS provide an efficient facility for a variety of modeling situations, for example:

- Simple site-scale problems using uniform flow and a few wells
- Regional modeling problems that cover very large regions
- “Screening” models that test conceptual models, as a preparatory step in the development of more complex numerical models.

Although MODAEM is currently limited to steady-state models of a single aquifer, it provides many powerful facilities for regional and local scale modeling. This introduction is intended for users who are new to the AEM. For a more detailed introduction to the AEM, see Analytic Element Modeling of Groundwater Flow (Haitjema, 1995); for a detailed explanation of the mathematics of the AEM, see Groundwater Mechanics (Strack, 1989).

A note to experienced AEM users

MODAEM in GMS differs from most analytic element codes (e.g. SLAEM, WhAEM for DOS/Windows, GFLOW, TimSL/TimML) in that the data input

is consistent with MODFLOW. This allows the GMS map coverages to be compatible with both MODAEM and MODFLOW models; in general, data will only need to be entered once for projects that use both codes. This has these important implications:

1. Flow rates for wells and discharge-specified line sinks follow the MODFLOW convention, which is that a pumping well has a *negative* discharge rate and an injection well has a *positive* discharge rate.
2. The “resistance” for rivers, drains, and GHBs has been replaced with a “conductance”, in a manner consistent with MODFLOW. For a river, the conductance is defined as $\tilde{c} = w \times k_c / t_c$ in units of $[L/T]$ where $\tilde{c}$ is the conductance, w is the stream width, k_c is the vertical hydraulic conductivity of the stream bed, and t_c is the thickness of the stream bed.
3. Aquifers can be *bounded*, just as in MODFLOW. The boundary is constructed of “left-discharge” line-sink elements, and continuity of flow is guaranteed within the closed domain. Currently, GMS supports discharge-specified and head-specified boundaries (MODAEM also supports general-head boundaries; these may be included in a future GMS release).

Experienced AEM users may wish to review the remainder of this section, however, if you are familiar with the proper use of AEM codes, you may skip to the next section.

3.1.2 What are analytic elements?

The AEM is based on the use of analytic solutions for problems in groundwater flow. For example, the potentiometric heads due to a well in two dimensions is shown in Figure 3-1(a) below.

Most analytic solutions may be *superimposed* to provide a solution for more complex problems, for example two wells pumping near one another (as shown in Figure 3-1(b) below).

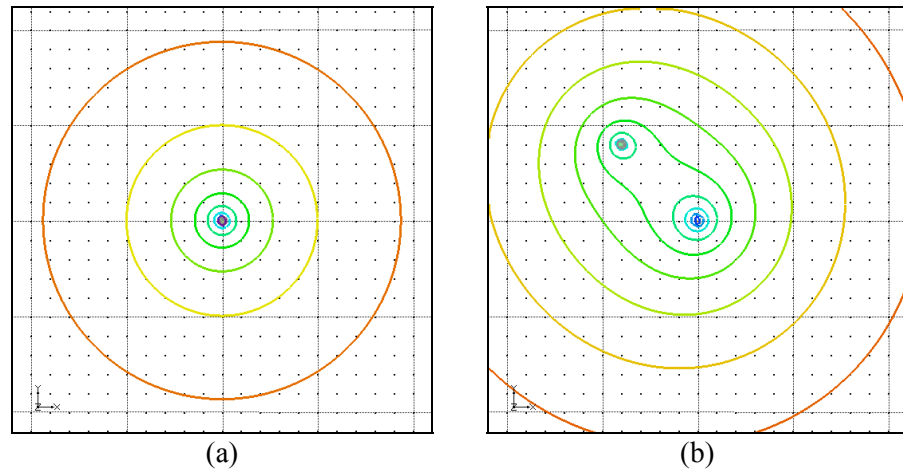


Figure 3-1 (a) Well (b) Two wells illustrating superposition

In addition to wells, MODAEM makes use of line-sink elements to represent surface waters or other linear infiltration features (Figure 3-2(a)), and area-sink elements for recharge from rainfall, infiltration ponds and other features (Figure 3-2(b)).

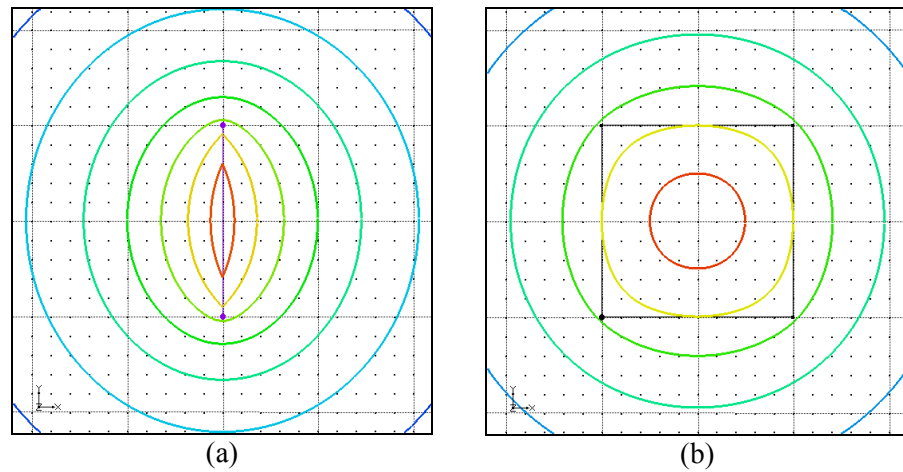


Figure 3-2 (a) Line-sink (b) Area-sink

Although MODAEM is limited to a single aquifer, the aquifer may be heterogeneous. The aquifer can be divided into sub-domains, with each sub-domain having a different hydraulic conductivity, base elevation, thickness, and/or porosity.

3.1.3 About the mathematics of analytic elements

It is not necessary for the new modeler to understand all of the mathematics behind the AEM. There is one important point to discuss in general terms: the discharge potential. MODAEM does not formulate the groundwater problem in terms of the potentiometric head, but instead in terms of a *discharge potential*, which combines the hydraulic conductivity, aquifer geometry, and head into one value. At any point in a MODAEM model, the discharge potential and the head are related by one of the following:

$$\Phi = K H \phi - \frac{1}{2} K H^2$$

for confined flow and

$$\Phi = \frac{1}{2} K \phi^2$$

for unconfined flow, where Φ is the discharge potential, ϕ is the head K is the hydraulic conductivity, and H is the aquifer height. For the case where $\phi = H$, the flow condition is just confined, and the two potential expressions are numerically equal. This allows MODAEM to simulate confined and unconfined flow in a regional model. The model is solved in terms of the potential, and either the confined or the unconfined expression is used to compute the head, depending on whether the potential is larger or smaller than the potential at the aquifer top.

For the modeler, this is the most important reason to understand that MODAEM uses discharge potentials. When you create an aquifer in MODAEM, the flow is confined whenever the head exceeds the aquifer top, automatically. To make a model where the flow is unconfined everywhere, specify an aquifer thickness such that the “aquifer top” is above the head everywhere in the model (or in a sub-domain).

Obviously, the ability to model confined and unconfined flow in the same model is one advantage, but discharge potentials also facilitate inhomogeneities (contrasts in aquifer properties). The discharge potential makes it possible to write an expression for the “jump” in the potential along the boundary of sub-domains (fortunately, the mathematics are omitted here!). However, this formulation is “non-linear” when the flow is unconfined on one or both sides of the sub-domain boundary; the model must do several iterations to ensure that the head is continuous across the boundary. In these cases, it is almost always necessary for the modeler to provide an initial guess for the average

head in the sub-domain; GMS provides an option (see below) for specifying this property.

3.1.4 Tips, tricks and suggestions

This section provides a few tips that will help the new AEM modeler. It is important to keep these points in mind when building your first MODAEM model.

Line sinks and resolution issues

In MODAEM, there are several applications of line-sink elements,

- Constant discharge line sinks
- Constant head line sinks
- Rivers (analogous to MODFLOW RIV)
- Drains (analogous to MODFLOW DRN)
- General-head boundaries (analogous to MODFLOW GHB)

In MODAEM, each line sink is a line segment along a path digitized by the user. Each segment has a *sink density*, which is the amount of water added to the aquifer or removed from the aquifer per unit length of the line segment. For constant discharge line sinks, GMS allows the modeler to enter either the total amount of water added to the aquifer for a string of line sinks, or the sink density to be applied to each line sink.

A common misconception for new AEM modelers arises with “constant head” line sinks. The term “constant head” does not mean that the head is actually the same everywhere along the element, but that MODAEM will compute a sink density for the line sink such that the specified head is matched exactly at the center of the element. For example, consider Figure 3-3(a) below, with a single constant head line sink with a head of 99 *m*.

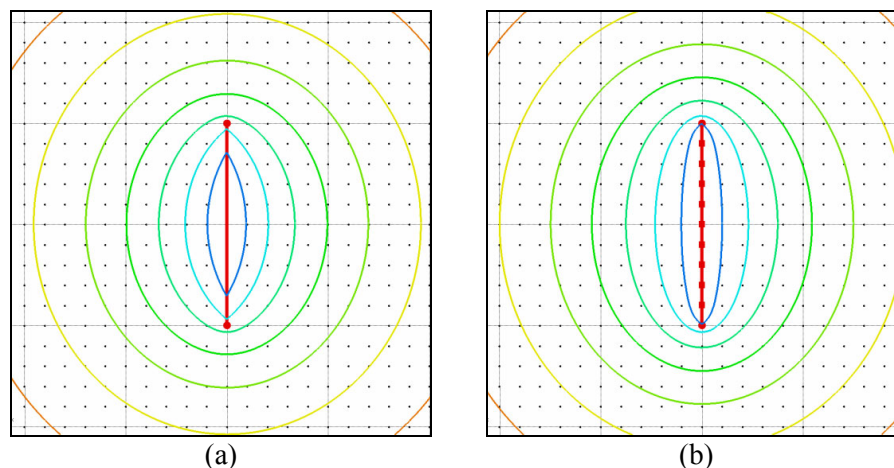


Figure 3-3 (a) Line-sink (b) Line-sink with extra vertices for better resolution

As you see, the head is matched only at the center of the element, and the heads vary along the single element. Now, see the result when the single specified-head line sink is replaced by ten line sinks as shown in Figure 3-3(b). This is clearly what the modeler intended; the head along the line sink *string* is 99 m.

It is up to the modeler to determine what resolution each string of line sinks needs for a particular problem (think of the length of line sinks in the same way you think of MODFLOW cell sizes). Fortunately, GMS provides a handy facility for adding and removing vertices along line segments, and adjusting the resolution along a string of elements.

The same rules apply for other line elements in MODAEM, including horizontal barriers and inhomogeneity boundaries. You will often wish to use GMS's "Distribute Vertices" command to ensure accurate solutions for heterogeneous aquifers.

Line sinks versus inhomogeneities

Recall from above that each line segment along a lone sink string has a constant sink density. If a string of line sinks crosses a sub-domain boundary, it is expected that there will be a "jump" in the sink density at the boundary. For an accurate solution, it is important to ensure that each segment of a line-sink string lies entirely within a single sub-domain. A correct arrangement is shown below. The inhomogeneity has a hydraulic conductivity 100 times larger than the outside conductivity, and the boundary of the inhomogeneity crosses the line-sink string at a vertex.

3.2 Description of Problem

This tutorial describes the use of GMS to model groundwater flow near the well field of Brazil, IN. Brazil (population 8188) operates a well field about 5

miles east of town, in the floodplain of Big Walnut Creek (see Figure 1). The objectives of this model are to:

1. Model the 5-year capture zone for the wellfield for use in the Brazil wellhead protection effort.
2. Examine the effects of the addition of an additional well to the wellfield.

The following figure shows the site location, along with the model boundaries.

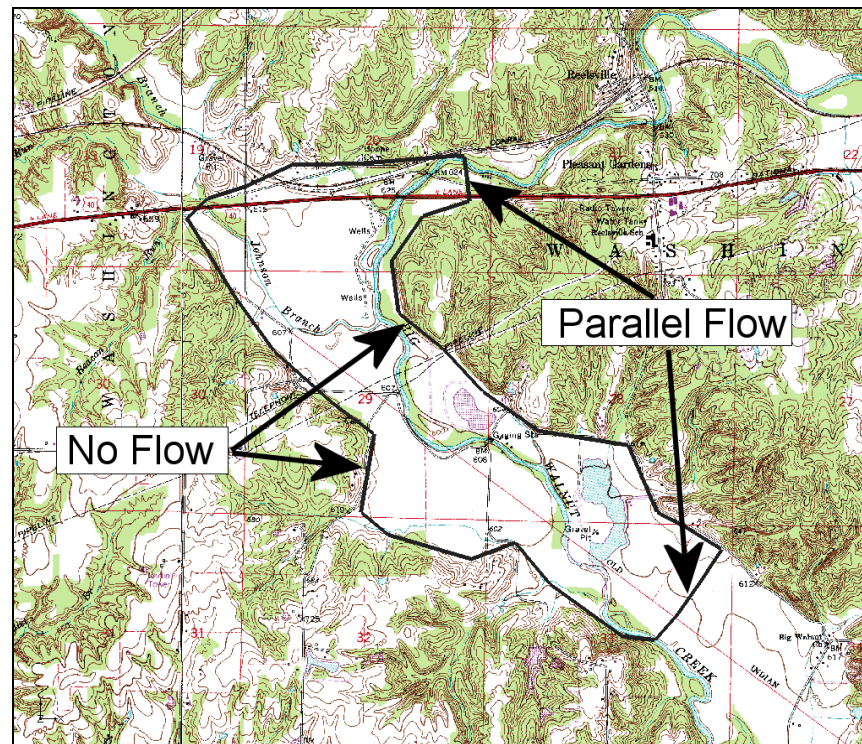


Figure 3-4 Model Boundary

3.2.1 Setting and Data Collection

The wellfield is situated in the floodplain of Big Walnut Creek. The aquifer is composed of coarse gravel with an average hydraulic conductivity of 250 ft/d (60.9 m/d), deposited in a buried bedrock valley. Although the bedrock surrounding the valley is slightly permeable, it is not considered an important source of water. The thickness of the gravel aquifer in the valley varies from 10 – 80 ft (3.0 – 24.4 m). At the wellfield, the ground elevation is roughly 600 ft (182.9 m), and the aquifer is roughly 60 ft (18.3 m) thick.

3.3 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

3.4 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Map
- MODAEM

You can see if these components are enabled by selecting the *File | Register* command.

3.5 Feature Objects

We are now ready to begin constructing the conceptual model. Conceptual models are constructed using feature objects in the *Map* module. Feature objects in *GMS* have been patterned after Geographic Information Systems (GIS) objects and include points, nodes, arcs, and polygons (Figure 3-5). Points are xy locations that are not attached to an arc. Points have unique ids and can be assigned properties. Points are typically used to represent wells. Arcs are sequences of line segments or edges which are grouped together as a single “polyline” entity. Arcs have unique ids and can be assigned properties. Arcs are grouped together to form polygons or are used independently to represent linear features such as rivers. The two end points of an arc are called “nodes” and the intermediate points are called “vertices”. Nodes have unique ids and can be assigned properties. Vertices are used solely to define the geometry of the arc. Polygons are a group of connected arcs that form a closed loop. A polygon can consist of a single arc or multiple arcs. If two polygons are adjacent, the arc(s) forming the boundary between the polygons is shared (not duplicated).

Feature objects are grouped into coverages. Each coverage represents a particular set of data.

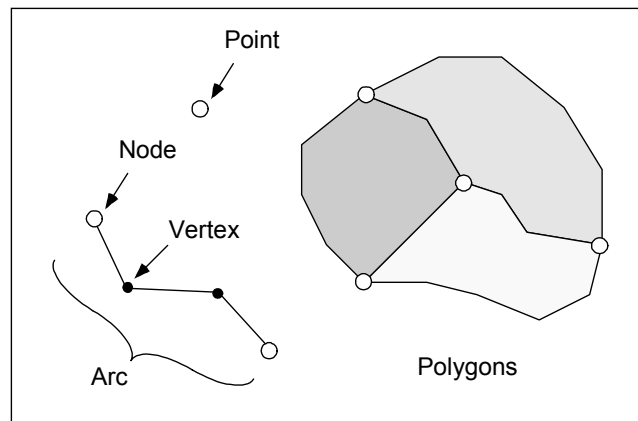


Figure 3-5 Feature Objects.

3.6 Reading in the Background Map

The first step to create our model is to read in a background image of the site we are modeling. We will use the image to guide us as we create points, arcs, and polygons to define features of our model.

1. Select the *Open* button .
2. Locate and open the directory entitled **tutfiles\modaem**.
3. Select and open the file **indiana.tiff**.

At this point the image registration dialog appears. If the image file had an associated world file or if the file contained a geo-reference then the registration dialog would not appear. This image file does not have any geo-referencing information so we will have to provide this information by identifying the real world coordinates at different points on the image.

4. In the *Register Image* dialog select the *Two Point Registration* option.
5. Position the red crosshairs as shown in the image below and enter the coordinates.
6. Select *OK* to exit the dialog.

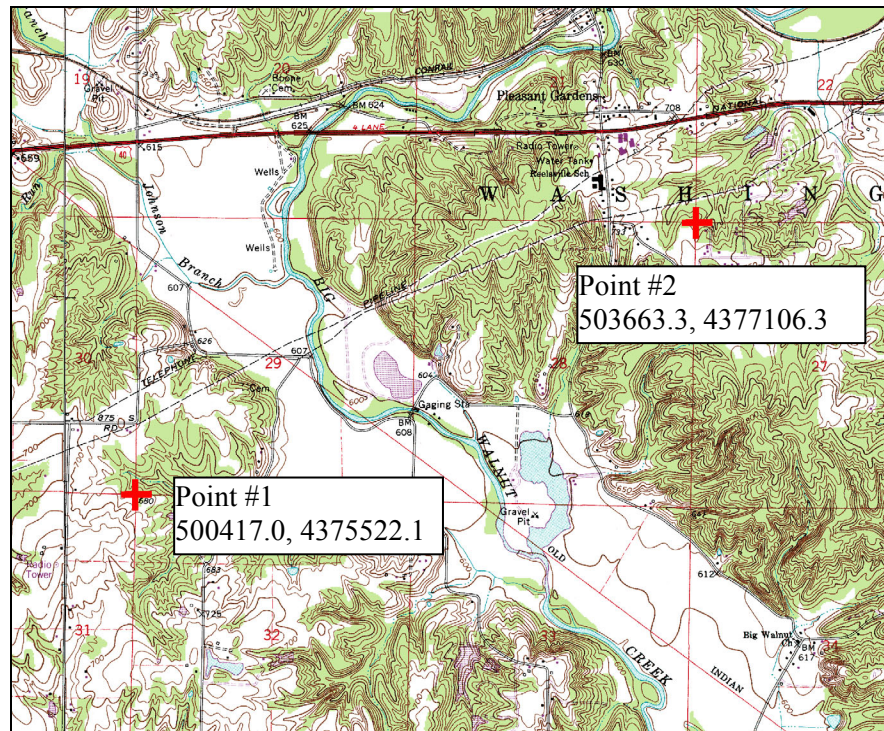


Figure 3-6 Image Registration

3.7 Defining the Units

At this point, we can also define the units used in the conceptual model. The units we choose will be applied to edit fields in the GMS interface to remind us of the proper units for each parameter.

1. Select the *Edit | Units* command.
2. For *Length*, select **m** (for meters). For *Time*, select **d** (for days). We will ignore the other units (they are not used for flow simulations).
3. Select the *OK* button.

3.8 Creating the Conceptual Model

We are now ready to enter our model data. First, we will create a MODAEM conceptual model. Then we will create coverages to define the boundary conditions and aquifer properties. The boundary of our model is shown in the following figure.

1. Switch to the *Map* module .

2. Right click on the **Map Data** folder in the *Data Tree* and select the *New Conceptual Model* option.
3. Change the name to **Indiana** and the model to **MODAEM** and click *OK*.
4. Right click on **Indiana** and select the *New Coverage* option.
5. Change the name to **Boundary** and select the *Use to define model boundary*. Click *OK*.
6. Select the Zoom tool .
7. Zoom in around the model area by dragging a box that encloses the area shown in Figure 3-7 below.
8. Select the *Create Arc* tool .
9. Click out the boundary as shown in Figure 3-7 below.

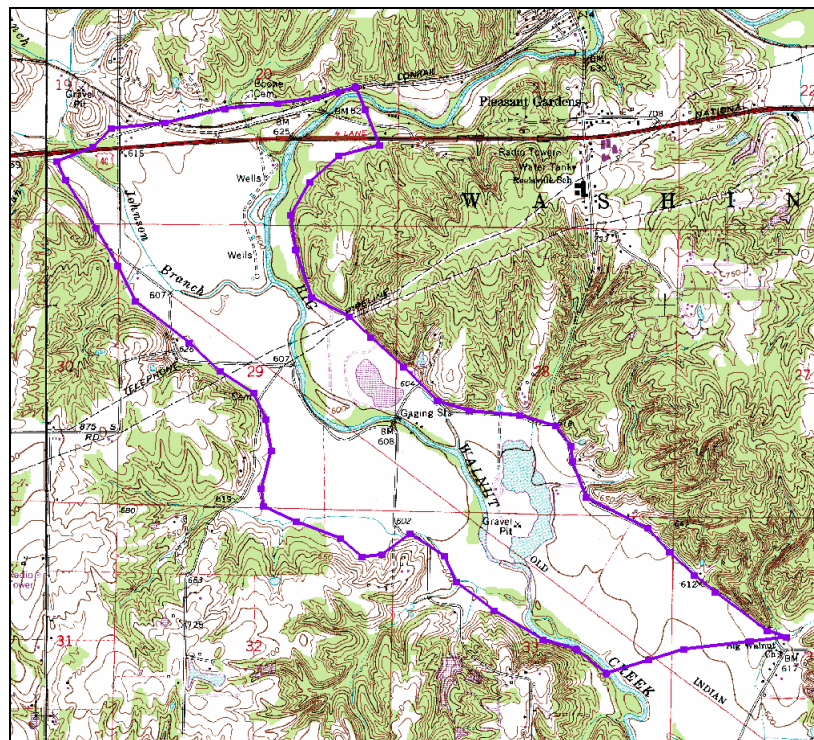


Figure 3-7 Boundary Arcs

3.9 Creating the Specified Head Arcs

By default, the arcs in a MODAEM boundary coverage are “no flow” boundaries. This means the arcs’ type is set to “specified flow” and the flow is set to 0. Next we will add specified head arcs to this coverage. To create the specified head arcs we will split the boundary arc into four separate arcs.

1. Select the *Select Vertices* tool .
2. Select the four vertices displayed in the figure below. To select more than one vertex, you must hold the shift key while selecting.

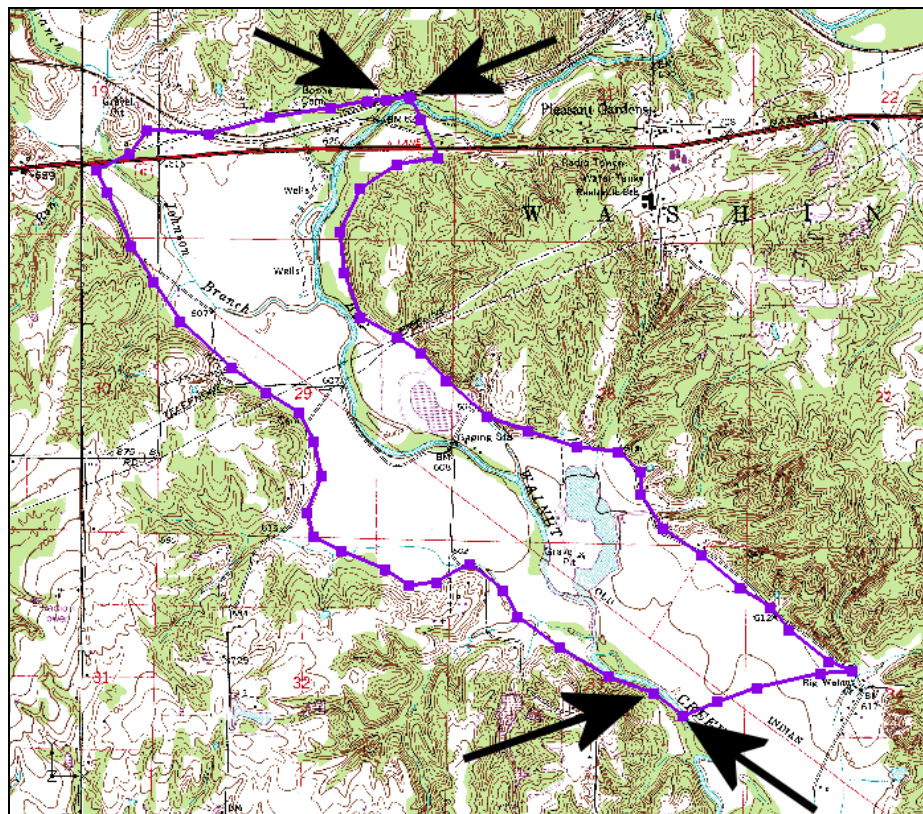


Figure 3-8 Convert Vertices to Nodes

You may need to insert additional vertices. This can be done by using the *Create Vertex* tool . Simply select the tool and then click on the arc in the location that you want the new vertex to be. Also, depending on how you created your boundary arc, one of the vertices shown in the figure above may actually be a node. In that case you will not be able to select it with the select vertex tool. If you do have a node at one of the locations shown above just select the other three vertices.

3. Once you have the vertices selected, select the *Feature Objects | Vertices <-> Nodes* command.

4. Select the *Select Arcs* tool .
5. Select the two new arcs that we created on the north and south of the boundary.

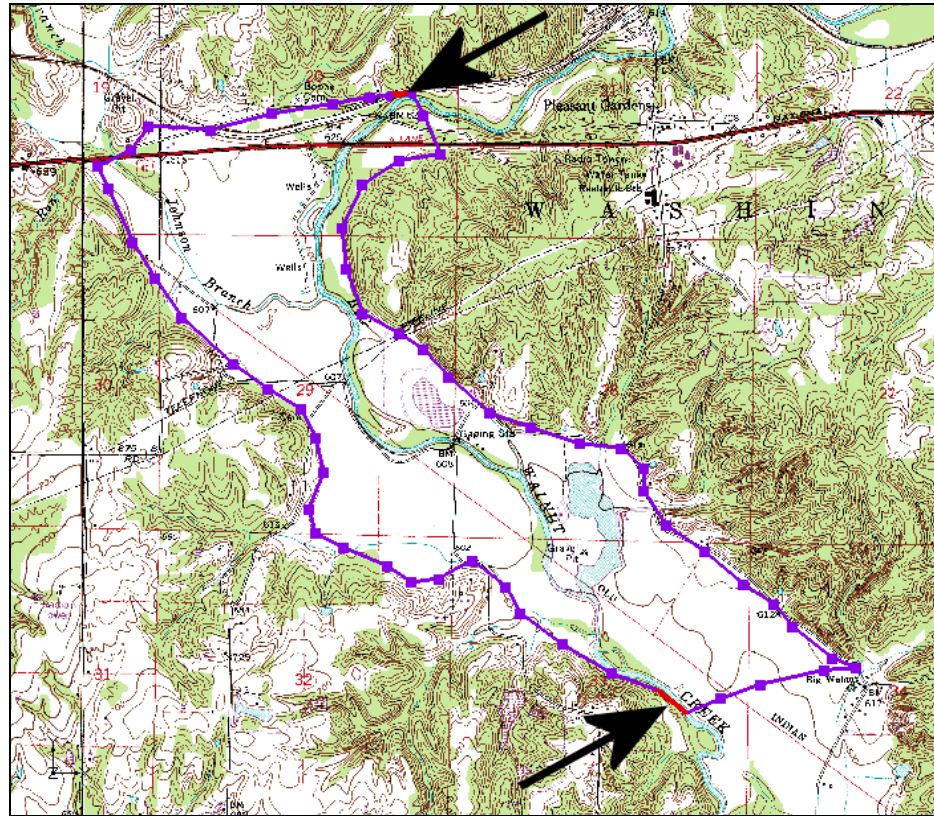


Figure 3-9 Specified Head Arcs

6. Select *Properties* button .
7. In the *All* row change the type to **spec. head**.
8. Select *OK* to exit the dialog.
9. Select the *Select Points/Nodes* tool .
10. Select both nodes on the northern specified head arc. To select more than one node, you can hold the shift key down while you click or you can drag a box around both nodes.
11. Select the *Properties* button .
12. In the *Head* field for both nodes enter **182.0**.

13. Repeat steps 10-12 for the nodes attached to the southern specified head arc and enter **178.6** for the head value.

3.10 Entering the Aquifer Properties

Next we will enter the properties of our aquifer. Aquifer properties can be assigned to individual polygons, and we can also define properties for a “background aquifer.”

1. Select the *MODAEM | Global Options* command.
2. In the *Background aquifer properties* section enter **170.0** for the *Base* and **60.0** for the *Hyd. cond.*
3. Select *OK* to exit the dialog.

With a boundary coverage we must also have a single polygon that defines the aquifer we are modeling.

4. Select the *Feature Objects | Build Polygons* command.

3.11 Saving the Project

We are now ready to run MODAEM. With other models in GMS, like MODFLOW for example, you must first save your changes to the project before you run the model. When you run MODAEM, however, the data currently in memory is written to temporary files that MODAEM reads to compute its solution. Therefore, you don’t have to save your changes in GMS before running MODAEM. However, it’s a good idea to save your work periodically anyway, so let’s do so now.

1. Select the *File | Save As* command.
2. Enter **brazil** as the name of the project.
3. Select the *Save* button.

Now you can hit the save button  periodically as you develop your model.

3.12 Running MODAEM

We are now ready to run MODAEM. This can be done by selecting the menu command *MODAEM | Solve* or by hitting the *F5* key. Once this command is executed a dialog will appear showing the output from the MODAEM model.

1. Hit the *F5* key.
2. When MODAEM is finished, select the *Close* button.

Head contours should now appear inside our boundary coverage.

3. Select the *Display Options* button .
4. Select the *MODAEM* tab.
5. Click on the *Options* button next to the *Contours* toggle.
6. Change the *Contour method* to **Linear and Color Fill**.
7. Under the *Line options* section, change the *Line style* so that the line color is black.
8. Under the *Fill options* section of the dialog change the *Transparency* value to **0.4**.
9. Select the *Color Ramp* button.
10. Under the *Palette Method* section of the dialog, turn on *Legend*.
11. Select *OK* repeatedly to close all of the dialogs.

3.13 Creating the River

Now we will add the river to our model.

1. Right click on **Indiana** in the *Data Tree* and select the *New Coverage* option.
2. Change the name of the coverage to **River**.
3. Under the *Source/Sink/BCs* section toggle on the **River** option.
4. Select **OK** to exit the dialog.
5. Select the *Create Arc* tool .
6. Click out the river arc starting near the northern specified head boundary and ending near the southern specified head boundary, as shown in Figure 3-10 below. Don't extend the river beyond the boundary coverage.

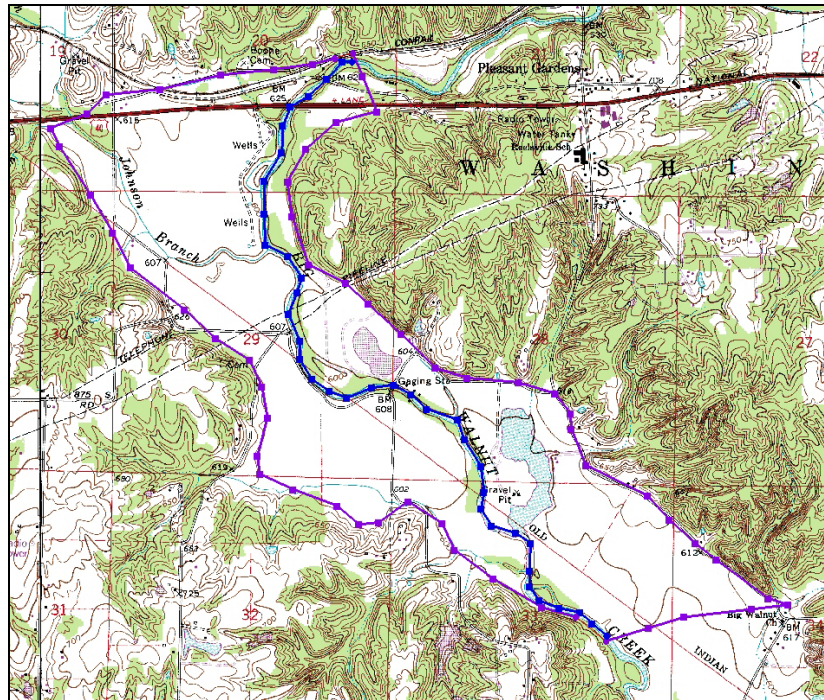


Figure 3-10 Modeling the River

7. Select the *Select Arcs* tool .
8. Click anywhere on the river arc to select it.
9. Select *Properties* button .
10. Change the type of the arc to **river**.
11. Enter a value of **5000.0** for the *Cond.* (conductance) and click *OK*.
12. Select the *Select Points/Nodes* tool .
13. Double click on the river node at the northern end of the model.
14. Enter **182.0** for the *Head* and **179.0** for the *Elev*.
15. Select *OK* to exit the dialog.
16. Repeat the same process for the southern river node and enter **178.6** for the *Head* and **175.6** for the *Elev*.

3.14 Running MODAEM

We are now ready to run MODAEM again.

1. Hit the *F5* key.
2. When MODAEM is finished, select the *Close* button.

You should notice some change in the head contours, particularly around the river arc.

3.15 Adding Recharge

Now we will add recharge to the model.

1. Right click on the **Boundary** coverage and select the *Duplicate* command.
2. Double click on the **Copy of Boundary** coverage.
3. Change the name to **Recharge**.
4. In the *Sources/Sinks/BCs* section of the dialog, toggle off *Specified Head* and *Specified Flow*.
5. In the *Areal Properties* section of the dialog, toggle on *Recharge*.
6. Select OK to exit the dialog.
7. Select the *Select Polygons* tool .
8. Double click on the polygon and assign a value of **.000418** to the *Recharge* field. Click *OK* to exit the dialog.

3.16 Running MODAEM

We are now ready to run MODAEM again.

1. Hit the *F5* key.
2. When MODAEM is finished, select the *Close* button.

3.17 Production Wells

Now we will import production wells from a tab delimited text file.

1. Right click on **Indiana** in the *Data Tree* and select the *New Coverage* option.

2. Change the name of the coverage to **Wells**.
3. Under the *Source/Sink/BCs* section toggle on the **Wells** option.
4. Select *OK* to exit the dialog.
5. Select the *Open* button .
6. Locate and open the directory entitled **tutfiles\modaem**.
7. Select and open the file **prod_wells.txt**.
8. Toggle on the *Heading row* toggle.
9. Click the *Next >* button.
10. Change the *GMS data type* to **Well data**.
11. In the *File preview* section of the dialog change the *Type* of the first column to **X**, the second to **Y**, and the third to **Flow Rate**.
12. Select the **Finish** button to exit the dialog.

You may have difficulty seeing the wells. The well symbol can be changed in the *Display Options* dialog by clicking on the *Display* macro .

3.18 Observation Wells

Before running MODAEM again we will also read in field measured head values.

1. Right click on **Indiana** in the *Data Tree* and select the *New Coverage* option.
2. Change the name of the coverage to **Observation**.
3. Under the *Observation Points* section toggle on the **Head** option.
4. Select *OK* to exit the dialog.
5. Select the *Open* button .
6. Locate and open the directory entitled **tutfiles\modaem**.
7. Select and open the file **well_head.txt**.
8. Toggle on the *Heading row* toggle.

9. Click the *Next >* button.
10. Change the *GMS data type* to **Observation data**.
11. In the *File preview* section of the dialog change the *Type* of the first column to **Name**, the second to **X**, the third to **Y**, and the fourth to **Obs. Head**.
12. Select the **Finish** button to exit the dialog.

3.19 Running MODAEM

We are now ready to run MODAEM again.

1. Hit the *F5* key.
2. When MODAEM is finished, select the *Close* button.

You should now see observation targets appear.

3.20 Conclusion

This concludes *MODAEM* tutorial. Here are the things that you should have learned in this tutorial:

- MODAEM is an analytic element model located in the Map module of GMS, and it uses only points, arcs, and polygons only to compute solutions.
- Images that do not come with registration information can be registered in GMS so that they are displayed in the appropriate location in your model coordinate system.
- The *Map* module is used to construct conceptual models using feature objects (points, arcs and polygons).
- Feature objects are grouped into coverages. There is always only one active coverage, and only the active coverage can be edited.

MODFLOW - Conceptual Model Approach

Two approaches can be used to construct a MODFLOW simulation in GMS: the grid approach or the conceptual model approach. The grid approach involves working directly with the 3D grid and applying sources/sinks and other model parameters on a cell-by-cell basis. The steps involved in the grid approach are described in the tutorial entitled *MODFLOW - Grid Approach*. The conceptual model approach involves using the GIS tools in the *Map* module to develop a conceptual model of the site being modeled. The location of sources/sinks, layer parameters such as hydraulic conductivity, model boundaries, and all other data necessary for the simulation can be defined at the conceptual model level. Once this model is complete, the grid is generated and the conceptual model is converted to the grid model and all of the cell-by-cell assignments are performed automatically. The steps involved in performing a MODFLOW simulation using the conceptual model approach are described in this tutorial.

It is recommended that you complete the *Interpolating Layer Elevations* and *MODAEM* tutorials before completing this tutorial.

4.1 Description of Problem

The problem we will be solving for this tutorial is illustrated in Figure 4-1a. The site is located in East Texas. We will assume that we are evaluating the suitability of a proposed landfill site with respect to potential groundwater contamination. The results of this simulation will be used as the flow field for

a particle tracking and a transport simulation in the MODPATH tutorial and the MT3DMS tutorial.

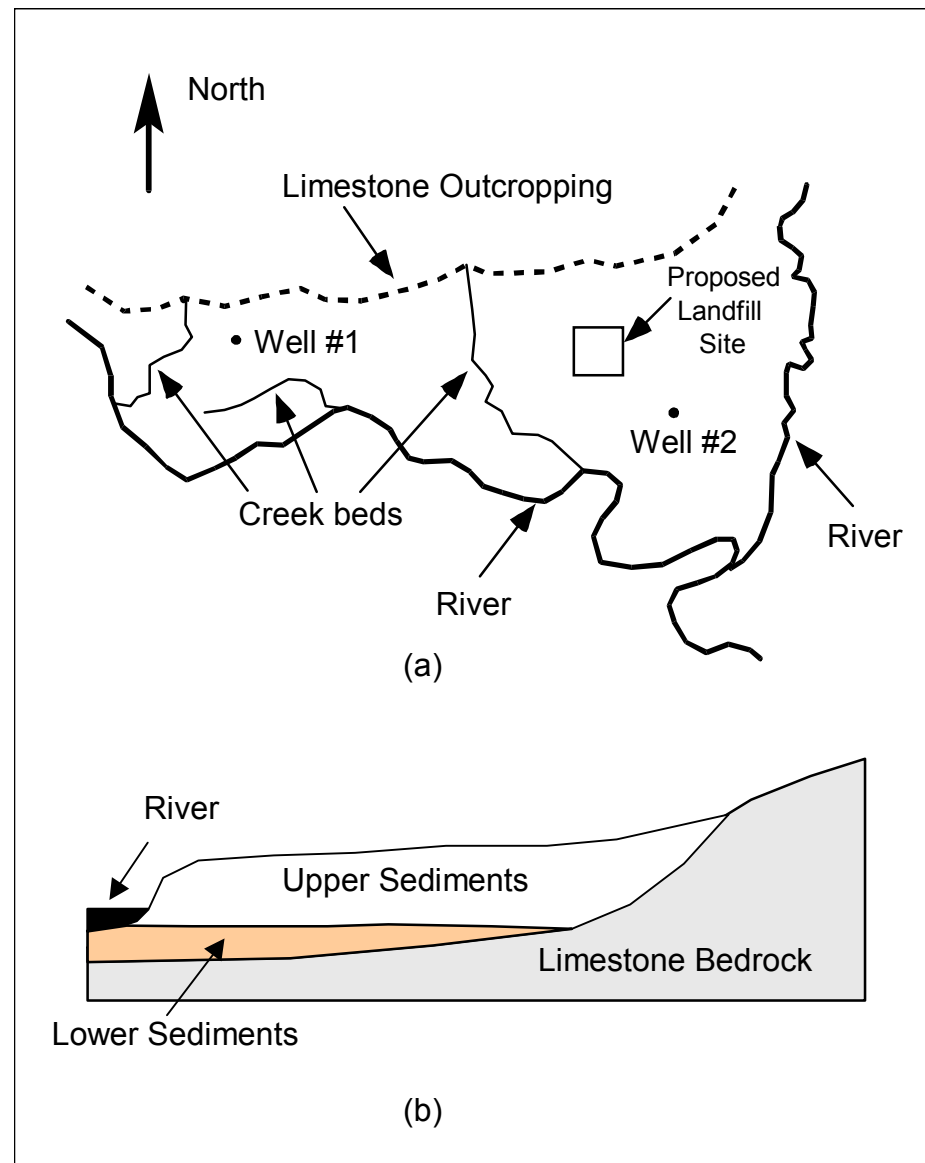


Figure 4-1 Site to be Modeled in This Tutorial. (a) Plan View of Site. (b) Typical North-South Cross Section Through Site.

We will be modeling the groundwater flow in the valley sediments bounded by the hills to the north and the two converging rivers to the south. A typical north-south cross section through the site is shown in Figure 4-1b. The site is underlain by limestone bedrock which outcrops to the hills at the north end of the site. There are two primary sediment layers. The upper layer will be modeled as an unconfined layer and the lower layer will be modeled as a confined layer.

The boundary to the north will be a no-flow boundary and the remaining boundary will be a specified head boundary corresponding to the average stage of the rivers. We will assume the influx to the system is primarily through recharge due to rainfall. There are some creek beds in the area which are sometimes dry but occasionally flow due to influx from the groundwater. We will represent these creek beds using drains. There are also two production wells in the area that will be included in the model.

NOTE: Although the site modeled in this tutorial is an actual site, the landfill and the hydrogeologic conditions at the site have been fabricated. The stresses and boundary conditions used in the simulation were selected to provide a simple yet broad sampling of the options available for defining a conceptual model.

4.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

4.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Geostatistics
- Map
- MODFLOW

You can see if these components are enabled by selecting the *File | Register* command.

4.4 Importing the Background Image

The first step in setting up the simulation is to import a digital image of the site being modeled. This image was created by scanning a portion of a USGS quadrangle map on a desktop scanner. The image was imported to GMS, registered, and a GMS project file was saved. To read in the image, we will open the project file. Once the image is imported to GMS, it can be displayed in the background as a guide for on screen digitizing and placement of model features.

4.4.1 Reading the Image

To import the image:

17. Select the *Open* button .
18. Locate and open the directory entitled **tutfiles\modfmap**.
19. Select the file entitled **start.gpr**.
20. Choose the *Open* button.

Now that the image is imported, it will appear each time the screen is refreshed. All other objects are drawn on top of the image. The image only appears in plan view.

4.5 Saving the Project

Before we make any changes, let's save the project under a new name.

4. Select the *File | Save As* command.
5. Enter **easttex** as the name of the project.
6. Select the *Save* button.

Now you can hit the save button  periodically as you develop your model.

4.6 Defining the Units

At this point, we can also define the units used in the conceptual model. The units we choose will be applied to edit fields in the GMS interface to remind us of the proper units for each parameter.

4. Select the *Edit | Units* command.
5. For *Length*, select **ft** (for feet). For *Time*, select **d** (for days). We will ignore the other units (they are not used for flow simulations).
6. Select the *OK* button.

4.7 Defining the Boundary

The first step is to define the outer boundary of the model. We will do this by creating an arc which forms a closed loop around the site.

4.7.1 Create the Coverage

1. Switch to the *Map* module .
2. Right click on the *Map Data* folder in the *Data Tree* and select the *New Conceptual Model* command.
3. For the *Name*, enter **East Texas**. For the *Model*, select **MODFLOW**.
4. Click *OK*.
5. Right click on the **East Texas** conceptual model and select the *New Coverage* command from the pop-up menu.
6. Change the *Coverage name* to **Boundary**. Change the *Default elevation* to **700**. Change the *Default layer range* to go from **1** to **2**.
7. Click *OK*.

4.7.2 Create the Arc

1. Select the *Create Arc* tool .
2. Begin the arc by clicking once on the left (west) side of the model at the location shown in Figure 4-2.
3. Create the arc by proceeding around the boundary of the site in a counter-clockwise direction and clicking on a sequence of points around the boundary. Don't worry about the spacing or the exact location of the points; just use enough points to define the approximate location of the boundary. The boundary on the south and east sides of the model should coincide with the rivers. The boundary along the top should coincide to the limestone outcropping as shown in Figure 4-2.
4. To end the arc, double click on the point where you began.

Note: As you are clicking on the points, if you make a mistake and wish to back up a point or two, press the *Backspace* key. If you wish to abort the arc and start over, press the *ESC* key.

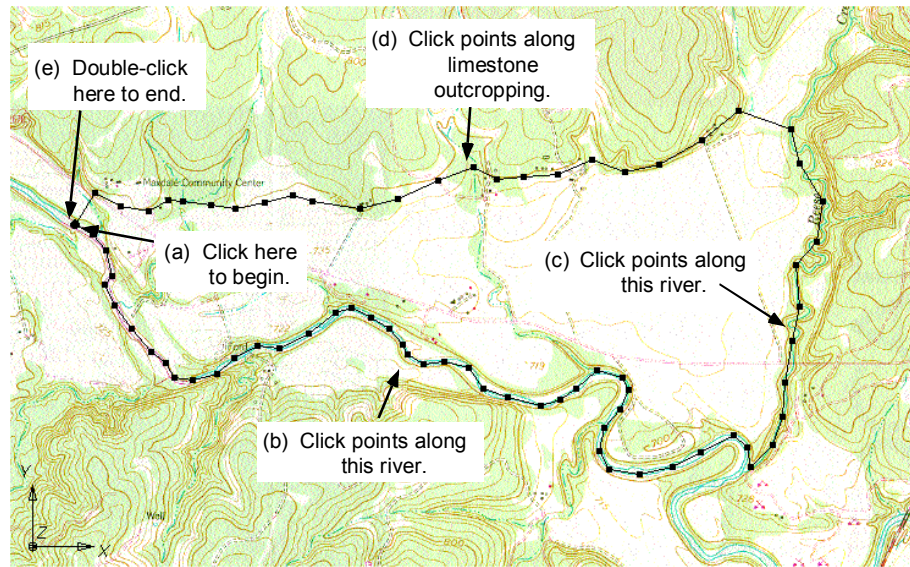


Figure 4-2 Creating the Boundary Arc.

4.8 Building the Local Source/Sink Coverage

The next step in building the conceptual model is to construct the local sources/sinks coverage. This coverage defines the boundary of the region being modeled and it defines local sources/sinks including wells, rivers, drains, and general head boundaries.

The properties which can be assigned to the feature objects in a coverage depend on the Conceptual model and the options set in the Coverage Setup dialog. Before creating the feature objects, we will change the options in the Coverage Setup dialog.

1. Right click on the **Boundary** coverage and select the *Duplicate* command from the pop-up menu. Change the new coverage name to **Sources/Sinks**.
2. Right-click on the **Sources/Sinks** coverage and select the *Coverage Setup* command from the pop-up menu.
3. For the *Preset*, select the **Source/sink coverage** option. This turns on a number of standard source/sink type properties.
4. In the list of *Sources/Sinks/BCs*, turn OFF the following options which we won't need for this tutorial:
 - *Specified Flow*
 - *General Head*
 - *River*
 - *Seepage Face*

- *Barrier*
5. Make sure the *Use to define model boundary (active area)* option is on.
 6. Click *OK*.

4.8.1 Defining the Specified Head Arcs

The next step is to define the specified head boundary along the south and east sides of the model. Before doing this, however, we must first split the arc we just created into three arcs. One arc will define the no-flow boundary along the top and the other two arcs will define the two rivers. An arc is split by selecting one or more vertices on the arc and converting the vertices to nodes.

1. Select the *Select Vertices* tool .
2. Select the two vertices shown in Figure 4-3. Vertex #1 is located at the junction of the two rivers. Vertex #2 is located at the top of the river on the east side of the model. To select both vertices at once, select the first vertex and then hold down the *Shift* key while selecting the other vertex.
3. Select the *Feature Objects | Vertices <-> Nodes* command.

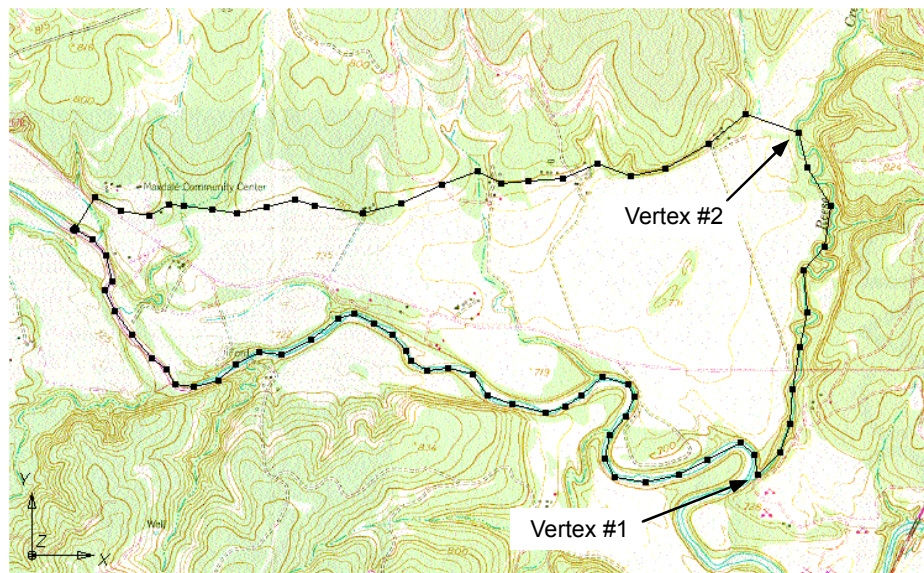


Figure 4-3 Convert Vertices to Nodes.

Now that we have defined the three arcs, we will specify the two arcs on the rivers as specified head arcs.

1. Select the *Select Arcs* tool .

2. Select the arcs on the south and east and (right and bottom) sides of the model by selecting one arc and holding down the *Shift* key while selecting the other arc.
3. Select *Properties* button .
4. Find the spreadsheet cell corresponding to the *All* row and the *Type* column. In this cell, select the **spec. head** type. This will change the types for both arcs.
5. Select the *OK* button.
6. Click anywhere on the model other than on the arcs to unselect them.

Note that the color of the arcs has changed indicating the type of the arc.

The next step is to define the head at the nodes at the ends of the arcs. The head along a specified head arc is assumed to vary linearly along the length of the arc.

1. Select the *Select Points/Nodes* tool .
2. Double click on the node on the west (left) end of the arc on the southern (bottom) boundary.
3. Enter a constant value of **697** for the *Head-Stage*.
4. Select the *OK* button.
5. In a similar fashion, assign a value of **685** to the node at the junction of the two rivers and a value of **703** to the node at the top of the arc on the east boundary of the model.

4.8.2 Defining the Drain Arcs

At this point, we will enter the arcs at the locations of the creek beds to define the drains.

1. Select the *Create Arc* tool .
2. Create the arc labeled as arc #1 in Figure 4-4. Start by clicking on the bottom arc, create the arc by clicking points along the creek bed, and end the arc by double clicking on the top arc.

Notice that when you click in the vicinity of a vertex on an existing arc or on the edge of an arc, GMS automatically snaps the arc you are creating to the existing arc and makes a node at the junction of the two arcs.

3. Create the arcs labeled arc #2 and arc #3 in Figure 4-4 the same way you made arc #1.

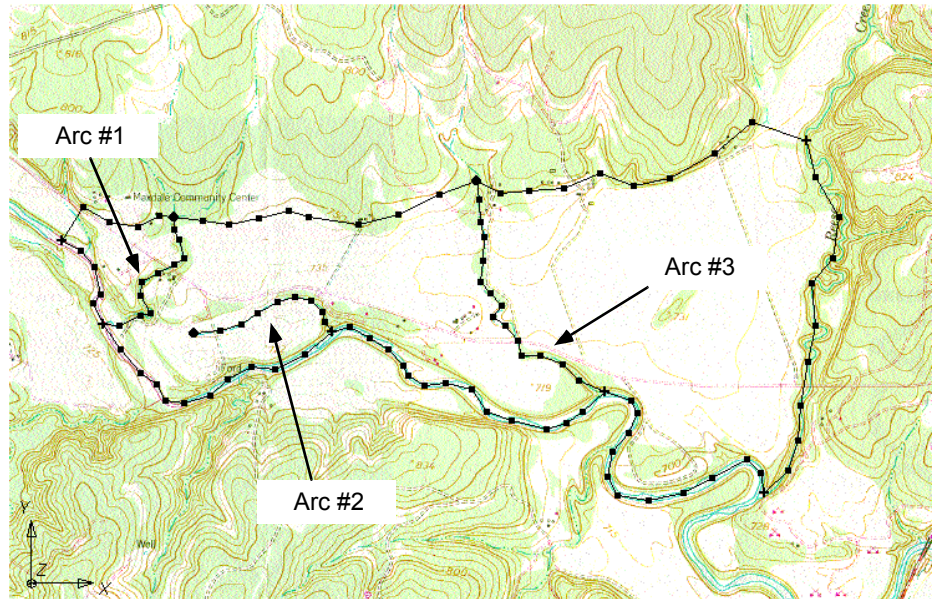


Figure 4-4 The Drain Arcs.

Next, we will define the arcs as drains and assign the conductance and elevation to the arcs.

1. Select the *Select Arcs* tool .
2. Select all of the drain arcs by clicking on the arcs while holding down the *Shift* key.
3. Select *Properties* button .
4. In the *All* row, *Type* column, select the **drain** option.
5. Enter a conductance of **6000** for all three arcs. This represents a conductance per unit length value. GMS automatically computes the appropriate cell conductance value when the drains are assigned to the grid cells.
6. Change the *From layer* and *To layer* properties to be **1** for each of the arcs. This means the drains will only be in layer 1 of the grid.
7. Select the *OK* button.

The elevations of the drains are specified at the nodes of the arcs. The elevation is assumed to vary linearly along the arcs between the specified values.

1. Select the *Select Points/Nodes* tool .
2. Double click on Node 2 in Figure 4-5. Notice that this node has 2 properties associated with it since it is attached to 2 arcs of different types.
3. Enter **696** for the *Bot. elev.* of the *drain* property. Do NOT change anything in the *spec. head* property. Click *OK*.
4. Repeat this procedure to assign the drain elevations to the nodes shown in Figure 4-5. Be sure to change the *drain* property only, and NOT the *spec. head* property.

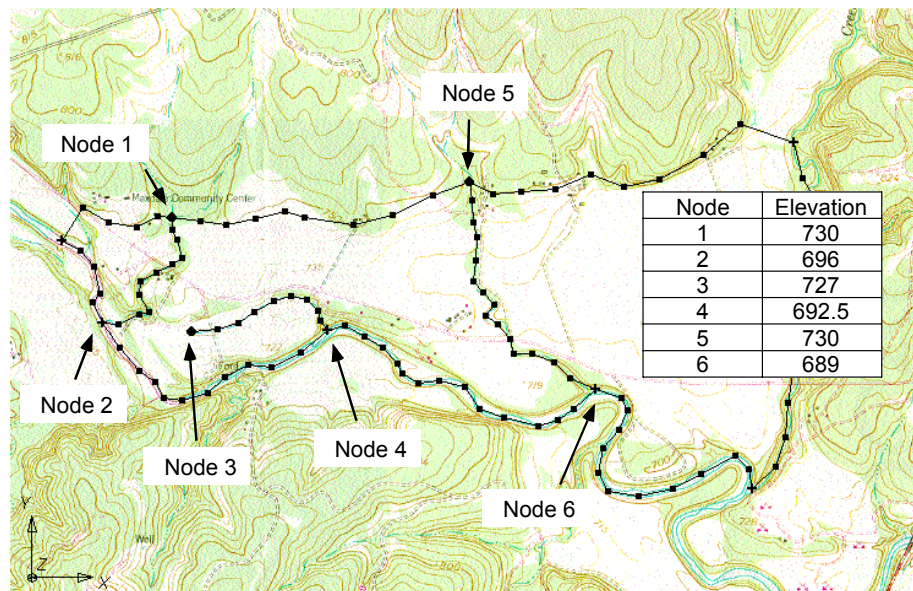


Figure 4-5 Elevations for Drain Nodes.

4.8.3 Building the polygons

With the local sources/sinks type coverage, the entire region to be modeled must be covered with non-overlapping polygons. This defines the active region of the grid. In most cases, all of the polygons will be variable head polygons (the default). However, other polygons may be used. For example, to model a lake, a general head polygon can be used. The simplest way to define the polygons is to first create all of the arcs used in the coverage and then select the *Build Polygons* command. This command searches through the arcs and creates a polygon for each of the closed loops defined by the arcs. These polygons are variable head by default but may be converted to other types by selecting the polygons and using the *Properties* command.

Now that all of the arcs in the coverage have been created, we are ready to construct the polygons. All of our polygons will be variable head polygons.

1. Select the *Feature Objects | Build Polygons* command.

Even though the polygons are created, there is no visible difference in the display. You can view the polygons if you wish by selecting the *Display | Display Options* command and turning on the *Polygons (Fill)* option.

4.8.4 Creating the Wells

The final step in creating the local sources/sinks coverage is to define the wells. Wells are defined as point type objects. Two wells will be created.

1. Select the *Create Point* tool .
2. Move the cursor to the approximate location of Well #1 shown in Figure 4-1 and click once with the mouse to create the point.
3. While the new point is selected, type the coordinates (**2741, 4673**) in the *X* and *Y* edit fields at the top of the GMS window and hit the *Tab* or *Enter* key.
4. Select *Properties* button .
5. For the *Type*, select the **well** option.
6. Enter a constant value of **-24100** for the flow (pumping) rate.
7. Change the *From layer* and *To layer* properties to be **1**. This means the well will only be in layer 1 of the grid.
8. Select the *OK* button.
9. In a similar fashion, create the other well at the location (**10557, 3290**) and assign a pumping rate of **-100,000**. However, for this well, change the *From layer* and *To layer* so that the well is applied only to layer two (change both the edit fields to **2**).

Grid Refinement

A well represents a point of convergence in the groundwater flow and causes steep gradients in the head near the well. In order to accurately model the flow near wells, the grid is typically refined in the vicinity of the wells. This type of refinement can be performed automatically in GMS by assigning refinement data directly to the wells in the conceptual model.

1. Select the *Select Points/Nodes* tool .
2. Select both wells by clicking on the wells while holding the *Shift* key.
3. Select *Properties* button .

4. Find the *Refine* column, and in the *All* row, turn on the toggle. This turns on refinement for both points.
5. Change the *Base size* to **75**, the *Bias* to **1.1** and the *Max size* to **500** for both points.
6. Click *OK*.

4.9 Delineating the Recharge Zones

The next step in constructing the conceptual model is to construct the coverage which defines the recharge zones. We will assume that the recharge over the area being modeled is uniform except for the landfill. The recharge in the area of the landfill will be reduced due to the landfill liner system.

4.9.1 Copying the Boundary

We'll create our recharge coverage by copying the boundary.

1. Right click on the **Boundary** coverage and select the *Duplicate* command from the pop-up menu. Change the name of the new coverage to **Recharge**.
2. Right click on the **Recharge** coverage and select the *Coverage Setup* command.
3. In the *Areal Properties* list, turn on the *Recharge rate* property.
4. Select the *OK* button.

4.9.2 Creating the Landfill Boundary

Next, we will create the arc delineating the boundary of the landfill. To do this, we will first create a closed loop in the form of a rectangle at the approximate location of the landfill. We will then edit the nodes and vertices so that the arc coincides precisely with the boundary of the landfill.

1. Select the *Create Arc* tool .
2. Create a rectangular polygon representing the landfill as shown in Figure 4-6. Don't worry about getting the exact coordinates at this point.

Now that the arc is created in the approximate location, we will edit the coordinates of the vertices and nodes to define the precise coordinates.

3. Select the *Select Vertices* tool .

4. Drag a box around the entire landfill polygon rectangle, thus selecting all the vertices.
5. Select the *Feature Objects | Vertices<->Nodes* command.
6. Select the *Select Points/Nodes* tool .
7. Select one of the nodes that at the corner of the rectangle.
8. While the node is selected, enter the exact coordinates of the node in the *Edit Window*. Select the *Tab* key after entering each coordinate value.

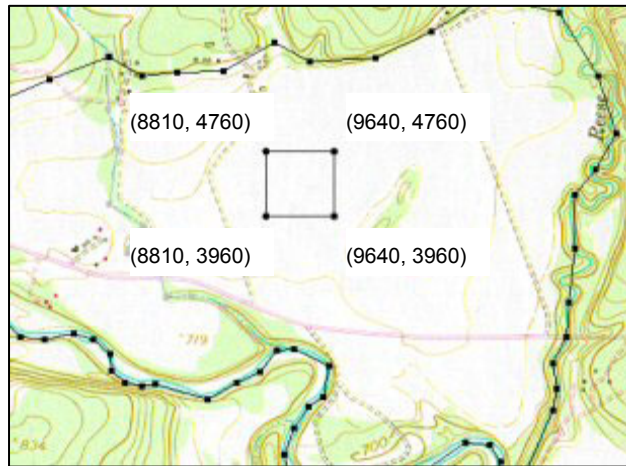


Figure 4-6 Landfill

9. Repeat this process for the remaining corners of the landfill polygon.

4.9.3 Building the Polygons

Now that the arcs are defined, we can build the polygons.

1. Select the *Feature Objects | Build Polygons* command in.

4.9.4 Assigning the Recharge Values

Now that the recharge zones are defined, we can assign the recharge values. We will assign one value to the landfill polygon, and another value to the remaining polygon.

1. Select the *Select Polygons* tool .
2. Double click on the landfill polygon.
3. Change the *Recharge rate* to **0.0002**.

Note: This recharge rate is small relative to the rate assigned to the other polygons. The landfill will be capped and lined and thus will have a small recharge value. The recharge essentially represents a small amount of leachate that escapes from the landfill.

4. Select the *OK* button.
5. Double click on the outer polygon.
6. Change the *Recharge rate* to **0.0228**.
7. Select the *OK* button.

4.10 Defining the Hydraulic Conductivity

Next we will enter the hydraulic conductivity for each layer. In many cases, you may wish to define multiple polygons defining hydraulic conductivity zones. For the sake of simplicity, we will use a constant value for each layer.

4.10.1 Copying the Boundary

We'll create our recharge coverage by copying the boundary.

1. Right click on the **Boundary** coverage and select the *Duplicate* command from the pop-up menu. Change the name of the new coverage to **Layer 1**.
2. Right click on the **Layer 1** coverage and select the *Coverage Setup* command.
3. In the *Areal Properties* list, turn ON the following options
 - *Horizontal K*
 - *Vertical anis.*
4. Change the *Default layer range* to go from **1** to **1**.
5. Select the *OK* button.
6. Right click on the **Layer 1** coverage and select the *Duplicate* command from the pop-up menu. Change the name of the new coverage to **Layer 2**.
7. Right click on the **Layer 2** coverage and select the *Coverage Setup* command.
8. Change the *Default layer range* to go from **2** to **2**.
9. Select the *OK* button.

4.10.2 Top Layer

First, we will assign a K value for the top layer.

1. Select the **Layer 1** coverage in the *Data Tree*.
2. Select the *Feature Objects | Build Polygons* command.
3. With the *Select Polygons* tool , double click on the polygon.
4. Change the *Horizontal K* to **16**.
5. Change the *Vertical anis.* to **4**.
6. Select the *OK* button.

4.10.3 Bottom Layer

For the bottom layer:

1. Select the **Layer 2** coverage in the *Data Tree*.
2. Select the *Feature Objects | Build Polygons* command.
3. Double click on the polygon
4. Change the *Horizontal K* to **32**.
5. Change the *Vertical anis.* to **4**.
6. Select the *OK* button.

This completes the definition of the coverages in the conceptual model. Before continuing to create the grid, we will make the sources/sinks coverage the active coverage.

7. Select the **Sources/Sinks** coverage in the *Data Tree*.

4.11 Locating the Grid Frame

Now that the coverages are complete, we are ready to create the grid. The first step in creating the grid is to define the location and orientation of the grid using the Grid Frame. The Grid Frame represents the outline of the grid. It can be positioned on top of our site map graphically.

1. Select the *Feature Objects | New Grid Frame* command.

2. Switch to the *Select Grid Frame* tool  and double-click on the grid frame.
3. For the Z coordinate, change the *Origin* to **550** and the *Dimension* to **200**. This provides a set of initial values for the MODFLOW layer elevation arrays. Later, we will interpolate the layer elevations
4. Select the *OK* button to exit the *Grid Frame* dialog.

4.12 Creating the Grid

Now that the coverages and the Grid Frame are created, we are now ready to create the grid.

1. Select the *Feature Objects | Map → 3D Grid* command.

Notice that the grid is dimensioned using the data from the Grid Frame. If a Grid Frame does not exist, the grid is defaulted to surround the model with approximately 5% overlap on the sides. Also note that the number of cells in the x and y dimensions cannot be altered. This is because the number of rows and columns and the locations of the cell boundaries will be controlled by the refine point data entered at the wells.

2. In the *Z-Dimension* change *Number cells* to **2**.
3. Select the *OK* button.

4.13 Defining the Active/Inactive Zones

Now that the grid is created, the next step is to define the active and inactive zones of the model. This is accomplished automatically using the information in the local sources/sinks coverage.

1. Select one of the polygons.
2. Select *Properties* button .
3. Confirm that the layer assignment is 1 to 2 and click *OK*.
4. Select the *Feature Objects | Activate Cells in Coverage(s)* command.

Each of the cells in the interior of any polygon in the local sources/sinks coverage is designated as active and each cell which is outside of all of the polygons is designated as inactive. Notice that the cells on the boundary are activated such that the no-flow boundary at the top of the model approximately coincides with the outer cell edges of the cells on the perimeter while the

specified head boundaries approximately coincide with the cell centers of the cells on the perimeter.

4.14 Initializing the MODFLOW Data

Now that the grid is constructed and the active/inactive zones are delineated, the next step is to convert the conceptual model to a grid-based numerical model. Before doing this, however, we must first initialize the MODFLOW data:

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | New Simulation* command.
3. Select the *OK* button.

4.15 Interpolating Layer Elevations

The final step before we save the model and run MODFLOW is to define the layer elevations and the starting head. Since we are using the LPF package, top and bottom elevations are defined for each layer regardless of the layer type. For a two layer model, we need to define a layer elevation array for the top of layer one (the ground surface), the bottom of layer one, and the bottom of layer two. It is assumed that the top of layer two is equal to the bottom of layer one.

The simplest way to define layer elevations is to import a set of scatter points defining the elevations and interpolate the elevations directly to the layer arrays. In some cases, this is done using one set of scatter points. In this case, we will use two scatter point sets: one for the ground surface and one for the elevations of the bottom of layer one and the bottom of layer two. It is often convenient to use two scatter point sets in this fashion due to the source of the points. Ground surface points are often digitized from a map while layer elevations typically come from borehole data.

Layer interpolation is covered in depth in the *Interpolating Layer Data* tutorial.

4.15.1 Importing the Ground Surface Scatter Points

The scatter points have already been read in because they were included in the project file that we read in the beginning. These points came from importing a text file as described in the *2D Geostatistics* tutorial. The scatter sets are hidden so we will unhide them so you can see them.

1. Switch to the *2D Scatter Point* module .

2. In the *Data Tree*, check the boxes next to the two scatter point sets named *terrain* and *elevs*.
3. Make the **terrain** scatter point set the active one by selecting it in the *Data Tree*.

A set of scatter point symbols should appear on the model.

4.15.2 Interpolating the Heads and Elevations

Next, we will interpolate the ground surface elevations and starting heads to the MODFLOW grid.

1. Select the *Interpolation | Interpolate → MODFLOW Layers* command in.

This is the dialog that allows you to tell GMS which data sets you want to interpolate to which MODFLOW arrays. The dialog is explained fully in the *Interpolating Layer Data* tutorial.

2. Check to make sure that the **ground_elev** data set and the **Starting Heads** array are highlighted, and click the *Map* button.
3. Check to make sure that the **ground_elev** data set and the **Top Elevations Layer 1** array are highlighted, and click the *Map* button.
4. Select the *OK* button to perform the interpolation.

4.15.3 Interpolating the Layer Elevations

To interpolate the layer elevations:

1. Select the **elevs** scatter point set to make it the active one in the *Data Tree*.
2. Select the *Interpolation | Interpolate → MODFLOW Layers* command.

GMS automatically mapped the **Bottom Elevations Layer 1** and **Bottom Elevations Layer 2** arrays to the appropriate data sets based on the data set name.

3. Select the *OK* button.

4.15.4 Adjusting the Display

Now that we are finished with the interpolation, we can hide the scatter point sets.

1. Uncheck the scatter point sets in the *Data Tree*.

We will also turn off the grid frame.

2. Switch to the *Map* module .
3. Select the *Display Options* button .
4. Turn off the *Grid frame* option.
5. Select the *OK* button.

4.15.5 Viewing the Model Cross Sections

To check the interpolation, we will view a cross section.

1. Switch to the *3D Grid* module .
2. Select a cell somewhere near the center of the model.
3. Select the *View J Axis* button .

To get a better view of the cross section, we will increase the z magnification.

1. Select the *Display | Settings* command.
2. Enter a value of **5** for the *Z magnification* factor.
3. Select the *OK* button.

You may wish to use the arrow buttons in the *Tool Palette* to view different columns in the grid.

Note that on the right side of the cross section, the bottom layer pinches out and the bottom elevations are greater than the top elevations. This must be fixed before running the model.

4.15.6 Fixing the Elevation Arrays

GMS provides a convenient set of tools for fixing layer array problems. These tools are located in the *Model Checker* and are explained fully in the *Interpolating Layer Data* tutorial.

1. Select the *MODFLOW | Check Simulation* command.
2. Select the *Run Check* button.
3. Select the *Fix Layer Errors* button at the top of the dialog.

Notice that many errors were found for layer two. There are several ways to fix these layers. We will use the *Truncate to bedrock* option. This option makes all cells below the bottom layer inactive.

4. Select the *Truncate to bedrock* option.
5. Select the *Fix Affected Layers* button (it does not matter which layer is selected, all layers that are affected will be fixed).
6. Select the *OK* button to exit the *Fix Layer Errors* dialog.
7. Select the *Done* button to exit the *Model Checker*.

Notice that the layer errors have been fixed. Another way to view the layer corrections is in plan view.

8. Switch to plan view by selecting the *View K Axis* button .
9. In the mini-grid display, select the down arrow  to view the second layer.

Notice that the cells at the upper (Northern) edge of the model in layer two are inactive.

10. Switch back to the top layer by selecting the up arrow .

4.16 Converting the Conceptual Model

We are now ready to convert the conceptual model from a high-level feature object-based definition to a grid-based MODFLOW numerical model.

1. Switch to the *Map* module .
2. Select the *Feature Objects | Map → MODFLOW / MODPATH* command.
3. Make sure the *All applicable coverages* option is selected and select *OK*.

Notice that the cells underlying the drains, wells, and specified head boundaries were all identified and assigned the appropriate sources/sinks. The heads and elevations of the cells were determined by linearly interpolating along the specified head and drain arcs. The conductances of the drain cells were determined by computing the length of the drain arc overlapped by each cell and multiplying that length by the conductance value assigned to the arc. In addition, the recharge and hydraulic conductivity values were assigned to the appropriate cells.

4.17 Checking the Simulation

At this point, we have completely defined the MODFLOW data and we are ready to run the simulation. Let's run the *Model Checker* to see if GMS can identify any mistakes we may have made (the *Model Checker* is explained in more detail in the *MODFLOW - Grid Approach* tutorial).

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | Check Simulation* command.
3. Select the *Run Check* button. There should be no errors.
4. Select the *Done* button to exit the *Model Checker*.

4.18 Saving the Project

Now we are ready to save the project and run MODFLOW.

1. Select the *Save* button .

Note: Saving the project not only saves the MODFLOW files but it saves all data associated with the project including the feature objects and scatter points.

4.19 Running MODFLOW

We are now ready to run MODFLOW.

1. Select the *MODFLOW | Run MODFLOW* command. At this point MODFLOW is launched and the *Model Wrapper* appears.
2. When the solution is finished, select the *Close* button.

4.20 Viewing the Head Contours

A set of contours should appear. To get better contrast between the contours and the background image, we will change the contour color to blue.

1. Select the *Data | Contour Options* command.
2. Click on the down arrow on the contour *Line style* button.
3. Select a dark blue color.
4. Select the *OK* button to exit the dialog.

To view the contours for the second layer:

1. Select the down arrow ↓ in the mini-grid display.
2. After viewing the contours, return to the top layer by selecting the up arrow ↑.

4.21 Viewing the Water Table in Side View

Another interesting way to view a solution is in side view.

1. Select the *Select Cell* tool .
2. Select a cell somewhere near the well on the right side of the model.
3. Select the *View J Axis* button .

Notice that the computed head values are used to plot a water table profile. Use the left and right arrow buttons in the mini-grid display to move back and forth through the grid. You should see a cone of depression at the well. When finished:

4. Select the *View K Axis* button .

4.22 Viewing the Flow Budget

The MODFLOW solution consists of both a head file and a cell-by-cell flow (CCF) file. GMS can use the CCF file to display flow budget values. For example, we may want to know if any water exited from the drains. This can be accomplished simply by clicking on a drain arc.

1. Switch to the *Map* module .
2. Choose the *Select Arcs* tool .
3. Click on the rightmost drain arc.

Notice that the total flow through the arc is displayed in the strip at the bottom of the window. Next, we will view the flow to the river.

1. Click on one of the specified head arcs at the bottom and view the flow.
2. Hold down the *Shift* key and select each of the specified head arcs.

Notice that the total flow is shown for all selected arcs. These same steps can be used to display flow through polygons such as recharge polygons. Flow for a set of selected cells can be displayed as follows:

1. Switch to the *3D Grid* module .
2. Select a group of cells by dragging a box around the cells.
3. Select the *Data | Flow Budget* command.

This dialog shows a comprehensive flow budget for the selected cells.

1. Select *Done* to exit the dialog.
2. Click anywhere outside the model to unselect the cells.

4.23 Conclusion

This concludes the *MODFLOW - Conceptual Model Approach* tutorial. Here are the things that you should have learned in this tutorial:

- A background image can be imported to help you construct the conceptual model.
- It is usually a good idea to define the model boundary in a coverage and copy that coverage whenever you need to create a new coverage.
- You can customize the set of properties associated with points, arcs and polygons by using the *Coverage Setup* dialog.
- Some arc properties, like head, are not specified by selecting the arc but by selecting the nodes at the ends of the arc. That way the property can vary linearly along the length of the arc.
- A grid frame can be used to position the grid, but is not required.
- You must use the *Map → MODFLOW / MODPATH* command every time you want to transfer the conceptual model data to the grid.
- You can specify things like layer elevations and hydraulic conductivities using polygons in the conceptual model, but that will result in stair-step-like changes. For smoother transitions, you can use 2D scatter points and interpolation.

MODPATH

This tutorial describes the steps involved in setting up a MODPATH simulation in GMS. MODPATH is a particle tracking code developed by the U.S. Geological Survey. MODPATH tracks the trajectory of a set of particles from user-defined starting locations using the MODFLOW solution as the flow field. The particles can be tracked either forward or backward in time. Particle tracking solutions have a variety of applications, including the determination of zones of influence for injection and extraction wells.

5.1 Description of Problem

The problem we will be solving for this tutorial is an extension of the problem described in the previous tutorial entitled MODFLOW - *Conceptual Model Approach*. If you have not yet completed the previous tutorial, you may wish to do so before continuing.

In the previous tutorial, a site in East Texas was modeled. We will be using the solution from this model as our flow field for the particle tracking simulation. The model includes a proposed landfill. For this tutorial, we will be performing two particle tracking simulations to analyze the long term effects of contamination from the landfill. First we will do reverse particle tracking from the well on the east side of the model to see if the zone of influence of the well overlaps the landfill. Then we will do forward tracking using an array of particles starting at the landfill to analyze the region of potential contamination for the landfill.

5.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

5.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW
- MODPATH

You can see if these components are enabled by selecting the *File | Register* command.

5.4 Importing the Project

The first step is to import the East Texas project. This will read in the MODFLOW model and solution, and all other files associated with the model.

To import the project:

1. Select the *Open* button .
2. In the *Open* dialog, locate and open the directory entitled **tutfiles\modfmap\sample**.
3. Select the file entitled **sample.gpr**.
4. Choose the *Open* button.

If the MODPATH component has been licensed and enabled, the MODPATH menu becomes available whenever you have a MODFLOW simulation in GMS. Thus, at this point we are ready to create particles. First, however, we will look at the porosity.

5.5 Assigning the Porosities

In order to calculate the tracking times, a porosity value must be defined for each of the cells in the grid. By default, GMS automatically assigns a porosity of 0.3 to all the cells in the grid. This value is acceptable so we don't need to do anything.

If we did want to change the porosity, we could do it in a number of ways. The first way is to assign porosities to the polygons in the conceptual model and selecting the *Map* → *MODFLOW / MODPATH* command. The second way is to select the *Porosity Array* command from the *MODPATH* menu in the 3D Grid module. This allows you to edit a spreadsheet of values. Another way is the select grid cells and use the *MODPATH | Porosity* command to edit the porosity of the selected cells.

5.6 Defining the Starting Locations

Now we need to specify the starting locations for the particles. We want to create a set of particle starting locations surrounding the cell containing the well on the east (right) side of the model.

To generate the starting locations:

1. Switch to the *3D Grid* module .
2. Select the *MODPATH | Generate Particles at Wells* command.
3. Make sure the number of particles is set to **20** and the *Extraction wells* option is selected.
4. Select the *OK* button.

A number of things happen now. GMS creates particles at every cell that contains a well. It then saves a set of MODPATH input files to a temporary folder and automatically runs MODPATH in the background. When MODPATH is done running, GMS reads in the pathlines that MODPATH computes. This all takes place very quickly – usually in a second or two.

You should now see a set of pathlines that converge on the east well. Notice that the pathlines intersect the area covered by the proposed landfill, indicating a potential for leachate from the landfill to appear in the water pumped from the well.

We are not interested in the well on the west (left) side of the model, so we will delete the particles and pathlines for that well.

1. Select the *Select Starting Locations* tool .
2. Drag a box surrounding the well on the west (left) side of the model.
3. Hit the *Delete* button.

5.6.1 Viewing the Pathlines in Cross Section View

The 3D nature of the pathlines is best seen in cross section view.

1. Select the *Select Cell* tool .
2. Select a cell near the right landfill.
3. Select the *View J Axis* button .

You may wish to move back and forth through the columns using the arrows   in the *Mini-grid plot*. When finished:

4. Select the *View K Axis* button .

5.7 Display Options

In addition to displaying the pathlines, GMS can draw a closed boundary around the pathlines connected to the well. This boundary is referred to as a “capture zone”. Capture zones can only be displayed if you are in plan view. GMS has a number of options for the display of pathlines and capture zones.

1. Select the *MODPATH | Display Options* command.
2. Turn on *Direction arrows*.
3. Make sure the *Boundary* option in the *Capture zones* section is turned on.
4. Turn on the *Poly fill* option in the *Capture zones* section.
5. Select the *OK* button.

You should now see arrows on the pathlines pointing in the direction of flow. You should also see the capture zone filled with a solid color.

5.8 Particle Sets

GMS organizes starting locations into “particle sets”. When we created the starting locations at the wells, GMS automatically created a particle set and put the new starting locations in it.

1. Expand the *Particle Sets* folder in the *Data Tree*.
2. Right-click on the particle set and select the *Properties* command from the pop-up menu.

5.8.1 Particle Sets Dialog

This brings up the *Particle Sets* dialog. Using the *Particle Sets* dialog you can change the particle set properties including the tracking direction, and the tracking duration.

One particle set is always designated as the active particle set. Whenever new points are created, they are added only to the active particle set. Similarly, you can only delete points from the active particle set.

By default, the tracking duration is set to track to the end, meaning, MODPATH will track the particles until they run into something (a sink, the edge of the model etc.). Let's change the tracking duration to a specific value.

1. In the *Track* column, switch the option to **Duration** in the pull-down list.
2. In the *Duration* column, change the value to **3,000**.
3. Click *OK*.

You should now see a smaller capture zone for the well.

5.8.2 Duplicating Particle Sets

Lets display a 3000 day capture zone, and a 1000 day capture zone. We'll turn the arrows off so they don't obscure the display of the capture zones.

1. Select the *MODPATH | Display Options* command.
2. Turn off the *Direction arrows* and click *OK*.

Now we will create another particle set by copying the existing one.

1. Using the *Data Tree*, change the name of the particle set to **3000 days** so that we know it goes for 3000 days.
2. Right-click on the particle set and select the *Duplicate* command from the pop-up menu.
3. Rename the new particle set **1000 days**.
4. Right-click on the 1000 days particle set and select the *Properties* command from the pop-up menu.
5. Change the *Duration* of the **1000 days** particle set to **1,000** and click *OK*.

5.8.3 Changing the Display Order

The order of the particle sets in the *Data Tree* is the order in which they are displayed. Thus, the particle sets listed on top in the spreadsheet will be displayed on top of the ones underneath. You can drag the particle sets up and down to change their order. Since the 1,000 day capture zone is smaller than the 3,000 day capture zone, we needed to make sure that it is displayed on top.

1. In the *Data Tree*, drag the *1,000 days* particle set up so it is above the *3,000 days* particle set.

You should now see two capture zones, the larger one being the 3,000 day capture zone, and the smaller one being the 1,000 day capture zone.

5.9 Tracking Particles from the Landfill

Next, we will perform forward tracking from a set of starting locations which coincide with the site of the proposed landfill.

5.9.1 Creating a New Particle Set

Create a new particle set for the particles we will create at the landfill.

1. In the *Data Tree*, right-click on the *Particle Sets* folder and select the *New Particle Set* command.
2. Change the name of the new particle set to **Landfill**.
3. Right-click on the *Landfill* particle set and select the *Properties* command.
4. Make sure the direction of the *Landfill* particle set is *Forward* and click *OK*.

5.9.2 Defining the New Starting Locations

Finally, we will create a new set of starting locations at the site of the proposed landfill. The particles will be placed on the top of the ground water table to simulate leachate entering from the surface.

We'll turn off the boundary fill option so we can see the new pathlines easier.

1. Select the *MODPATH | Display Options* command.
2. In the *Capture zones* section, turn off the *Poly fill* option.
3. Select the *OK* button.

Before selecting the cells, we will make the recharge coverage the active coverage so that the landfill polygon is clearly visible.

1. Switch to the *Map* module .
2. In the *Data Tree*, expand the *MODFLOW* conceptual module and select the *Recharge* coverage.

To select the cells:

1. Switch back to the *3D Grid* module .
2. Select the *Select Cells* tool .
3. Select the cells covered by the landfill by dragging a rectangle that coincides with the landfill boundary.
4. Select the *MODPATH | Generate Particles at Selected Cells* command.
5. Select the *OK* button.

Now you should see a set of pathlines starting at the landfill and terminating in the well, the creek bed, and in the river at the bottom of the model. If none of your landfill pathlines go to the well, you may need to add particles to the column of cells just to the right of the cells you currently have particles in. You may wish to view this solution in cross section view as well.

6. Click anywhere outside the grid to unselect the cells.

5.10 Color by Zone Code

Some of the pathlines that start at the landfill should terminate at the well. We want to easily identify these so we will make them a different color.

First, we'll turn off the display of the particles coming from the well.

1. In the *Data Tree*, turn off the display of the **1,000 days** and **3,000 days** particle sets by unchecking them.

Now we'll change the zone code for the cell containing the well.

2. Select the *Decrement* button  in the *Mini-Grid Plot* to view layer 2 of the grid.
3. With the *Select Cells* tool , select the cell with the well in it. You may need to zoom in to do this.
4. Select the *MODPATH | Cell Properties* command.

5. Change the *Zone code* to **2** and click *OK*.
6. Select the *MODPATH | Display Options* command.
7. In the *Color* pull-down list, change the selection to **Ending code**.
8. Select the OK button.

The pathlines that go from the landfill to the well should now be drawn in a different color.

5.11 Pathline Length/Time

One reason to do particle tracking is to find out how long it will take for particles to travel from one place to another. In this case we want to know how long it will take for particles to travel from the landfill to the well. GMS reports the length and travel time of selected pathlines.

1. Switch to the *Select Starting Locations* tool .
2. Click on one of the pathlines that goes from the landfill to the well.

In the status bar at the bottom of the GMS window, you should see some statistics for the selected pathline. One of the items is the time. We want to know the minimum time. We could click on different pathlines one at a time and compare their times, but there's an easier way.

3. Select all the pathlines that go from the landfill to the well by dragging a box around their starting locations (you may need to zoom in to do this).

In the status bar at the bottom of the GMS window, you should see the maximum and minimum lengths and times for all the selected pathlines.

5.12 Capture Zones by Zone Code

Notice that there is no closed boundary surrounding the pathlines originating from the landfill. By default, GMS only identifies capture zones for particles originating from wells. However, capture zones can be associated with particles originating from all cells with the same zone code. This feature can be used to group several wells together in the same capture zone. For example, if there were several wells located close together in a well field, you might want to know what the combined capture zone is for all the wells.

We can also use this feature to show the “capture zone” for the landfill.

1. Select the *MODPATH | Display Options* command.

2. Select the *Delineate by zone code* option in the *Capture Zones* section.
3. Turn on the *Poly fill* option.
4. Select the *OK* button.

You should now see the capture zone for the landfill pathlines. Notice that the capture zone includes areas where there are no pathlines. To fix this:

1. Select the *MODPATH | Display Options* command.
2. Change the *Thin triangle ratio* to **0.85** and select the *OK* button.

Notice how the boundary of the capture zone has been “sucked in” so that it corresponds more closely to the pathlines. This is what the *Thin triangle ratio* does. If you decrease it too much, the capture zone will begin to look bad. The default was appropriate for the well capture zone we saw earlier, but not for the landfill capture zone. You will sometimes have to adjust this value to get a good looking capture zone.

5.13 Conclusion

This concludes the *MODPATH* tutorial. Here are the things that you should have learned in this tutorial:

- *MODPATH* is available whenever a *MODFLOW* model is in memory. *MODPATH* requires a flow solution before pathlines can be computed.
- Unlike most models in *GMS*, *MODPATH* is much more automated, and *GMS* runs *MODPATH* behind the scene as soon as starting locations are created.
- You can create particle starting locations in two ways using either the *Generate Particles at Wells* or *Generate Particles at Selected Cells* commands.
- Particles are grouped into particle sets. You use particle sets to control the tracking direction, the duration, and the display order.
- There are a number of different display options available for pathlines, including displaying arrows, coloring by zone code, and displaying filled polygons representing capture zones (in plan view only).

MT3DMS - Grid Approach

This tutorial describes how to perform an MT3DMS simulation within GMS. An MT3DMS model can be constructed in GMS using one of two approaches: the conceptual model approach or the grid approach. With the conceptual model approach, the sources/sinks and zones in the model are defined with GIS objects and automatically assigned to the grid. With the grid approach, values are manually assigned to the grid. While the conceptual model approach is generally preferable for large, complicated models, simple models can be easily constructed using the grid approach. The grid approach is described in this tutorial.

6.1 Description of Problem

The problem to be solved in this tutorial is shown in Figure 6-1. This problem corresponds to the sixth sample problem ("Two-Dimensional Transport in a Heterogeneous Aquifer") described in the MT3DMS documentation. The problem consists of a low K zone inside a larger zone. The sides of the region are no flow boundaries. The top and bottom are constant head boundaries that cause the flow to move from the top to the bottom of the region. An injection well with a specified concentration provides the source of the contaminants. A pumping well serves to withdraw contaminated water migrating from the injection well. A steady state flow solution will be computed and a transient transport simulation will be performed over a one year period.

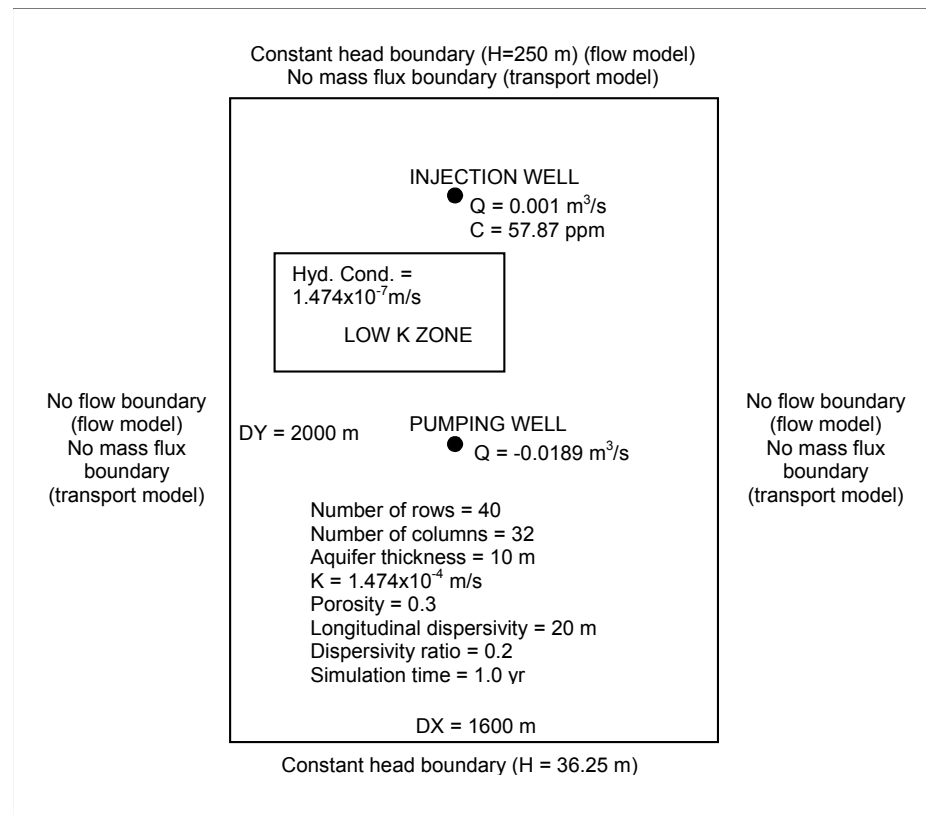


Figure 6-1 Sample Flow and Transport Problem.

6.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

6.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- MODFLOW
- MT3DMS

You can see if these components are enabled by selecting the *File | Register* command.

6.4 The Flow Model

Before setting up the MT3DMS simulation, we must first have a MODFLOW simulation. The MODFLOW solution will be used as the flow field for the transport simulation. In the interest of time, we will read in a previously created MODFLOW simulation.

1. Select the *Open* button .
2. Locate and open the directory entitled **tutfiles\mt3dgrid**.
3. Change the *Files of type* selection to **Model Super Files**.
4. Select the file entitled **flowmod.mfs**.
5. Choose the *Open* button.

Now we'll save our project under a new name. Since we're changing the name, we will run MODFLOW to compute solution files with the new name. Otherwise, when MT3D runs it will look for solution files with the new name and not find any.

6. Select the *File | Save As* command.
7. Locate and open the directory entitled **tutfiles\mt3dgrid**
8. Change the file name to **transport.gpr** and click *Save*.
9. Switch to the *3D Grid* module .
10. From the *MODFLOW* menu, select the *Run MODFLOW* command.
11. When it finishes running, select the *Close* button.

6.5 Building the Transport Model

Now that we have a flow solution, we are ready to set up the MT3DMS transport simulation. Like MODFLOW, MT3DMS is structured in a modular fashion and uses a series of packages as input. Consequently, the GMS interface to MT3DMS is similar to the interface to MODFLOW and we will follow a similar sequence of steps to enter the input data.

6.5.1 Initializing the Simulation

First, we will initialize the MT3DMS simulation.

1. Select the *MT3D | New Simulation* command.

6.5.2 The Basic Transport Package

The MT3DMS Basic Transport package is always required and it defines basic information such as stress periods, active/inactive regions, and starting concentration values.

Species

Since MT3DMS is a multi-species model, we need to define the number of species and name each species. We will use one species named “tracer.”

1. Select the *Define Species* button.
2. Select the *New* button.
3. Change the name of the species to **tracer**.
4. Select the *OK* button.

Packages

Next, we will select which packages we wish to use.

1. Select the *Packages* button.
2. Turn on the following packages:
 - *Advection Package*
 - *Dispersion Package*
 - *Source/Sink Mixing Package*
3. Select the *OK* button.

Stress Periods

The next step is to set up the stress periods. The flow simulation was steady state but the transport simulation will be transient. We will run the simulation for a one year time period. To do this we will use a single stress period (since the input values are constant) and allow MT3DMS to determine the appropriate transport step size.

1. Select the *Stress Periods* button.
2. Change the *Length* field to **365**.
3. Make sure the value in the *Trans. step size* is **0.0**. A value of zero signifies that *MT3DMS* will automatically compute the appropriate transport step size.
4. Select the *OK* button to exit the *Stress Periods* dialog.

Output Control

Next, we will specify the output options.

1. Select the *Output Control* button.
2. Select the *Print or save at specified interval* option.
3. Change the specified interval to **10**. This will output a solution at every tenth transport step.
4. Select the *OK* button to exit the *Output Control* dialog.

ICBUND Array

The ICBUND array is similar to the IBOUND array in MODFLOW. The ICBUND array is used to designate active transport cells ($ICBUND > 0$), inactive transport cells ($ICBUND = 0$), and constant concentration cells ($ICBUND < 0$). In most problems, ICBUND will be similar to IBOUND but it will differ. Typically, the cells which are constant head cells in the flow solution are not constant concentration cells in the transport solution. For our problem, all of the cells are active, therefore, no changes are necessary.

Starting Concentration Array

The starting concentration array defines the initial condition for the contaminant concentration. In our problem, the starting concentrations are all zero and the default is adequate.

HTOP and Thickness Arrays

MT3DMS uses the HTOP array and a thickness array to determine the layer geometry. However, the values for these arrays are determined by GMS automatically from the MODFLOW layer data and no input is necessary.

Porosity Array

Finally, we will define the porosity for the cells. Our problem has a constant porosity of 0.3. This is the default value in GMS so no changes need to be made.

This completes the definition of the Basic Transport package data.

1. Select the *OK* button to exit the *Basic Transport Package* dialog.

6.5.3 The Advection Package

The next step is to enter the data for the Advection package. We want to use the *Third Order TVD scheme (ULTIMATE)* solution scheme. This is the default, so we don't need to do anything.

6.5.4 The Dispersion Package

Next, we will enter the data for the Dispersion package.

1. Select the *MT3D | Dispersion Package* command.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant* → *Grid* option.
4. Enter a value of **20**.
5. Select the *OK* button.
6. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
7. Enter a value of **0.2** for the *Ratio of transverse dispersivity to longitudinal dispersivity* parameter.
8. Enter a value of **0.2** for the *Ratio of vertical dispersivity to longitudinal dispersivity* parameter.
9. Select the *Close* button to exit the *Dispersion Package* dialog.

6.5.5 The Source/Sink Mixing Package

Finally, we must define the data for the Source/Sink Mixing package. For our problem, we only have one source/sink: the injection well. To define the source at the injection well, we need to select the well and assign a concentration.

1. Select the cell containing the injection well (the upper well) by clicking anywhere in the interior of the cell.
2. Select the *MT3D | Point Sources/Sinks* command.
3. Turn on the *Well* option.
4. Enter a value of **57.87** for the concentration.
5. Select the *OK* button.
6. Click outside the grid to unselect the cell.

6.5.6 Saving the Simulation and Running MT3DMS

We are now ready to save the simulation and run MT3DMS.

1. Select the *Save* button .

2. Select the *MT3D | Run MT3DMS* command.
3. When the simulation is finished, select the *Close* button.

6.5.7 Changing the Contouring Options

When displaying plume data, the color fill option often provides excellent results.

1. Select the *Data | Contour Options* command.
2. Change the *Contour method* to **Color Fill**.
3. Select the *OK* button.

6.5.8 Setting Up an Animation

Finally, we will observe how the solution changes over the one year simulation by generating an animation. To set up the animation:

1. Select the *Display | Animate* command.
2. Make sure the *Data set* option is on and click *Next*.
3. Turn on the *Display clock* option.
4. Select the *Use constant interval option* and change the *Time interval* to **36.5**. This will result in 11 frames.
5. Select the *Finish* button.

You should see some images appear on the screen. These are the frames of the animation which are being generated.

1. After viewing the animation, select the *Stop*  button to stop the animation.
2. Select the *Step*  button to move the animation one frame at a time.
3. You may wish to experiment with some of the other playback controls. When you are finished, close the window and return to GMS.

6.6 Conclusion

This concludes the *MT3DMS – Grid Approach* tutorial. Here are the things that you should have learned in this tutorial:

- MT3D is available only if a MODFLOW model is in memory.
- MT3D relies on the MODFLOW solution files, so if you move or rename your MODFLOW files, you will probably need to regenerate the MODFLOW solution files so MT3D can find them.
- GMS gives MT3D the top and bottom elevation data it requires for each layer from the MODFLOW model.
- You can use the *Animation Wizard* to create an animation in GMS.

MT3DMS - Conceptual Model Approach

MT3DMS simulations can be constructed using either the grid approach where data are entered on a cell-by-cell basis or using the conceptual model approach where the data are entered via points, arcs, and polygons. The previous tutorial described how to use the grid approach. This tutorial describes how to use the conceptual model approach.

7.1 Description of Problem

The problem we will be solving for this tutorial is an extension of the problem described in the tutorial entitled *MODFLOW - Conceptual Model Approach*. Thus, if you have not yet completed the MODFLOW tutorial, you may wish to do so now before continuing.

In the MODFLOW tutorial, a site in East Texas was modeled. We will be using the solution from this model as the flow field for the transport simulation. The model included a proposed landfill. For this tutorial, we will be performing two transport simulations to analyze the long term potential for migration of leachate from the landfill. In the first simulation, we will be modeling transport due to advection and dispersion only. In the second simulation, we will include sorption and decay in addition to advection.

7.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

7.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW
- MT3DMS

You can see if these components are enabled by selecting the *File | Register* command.

7.4 Importing the Project

The first step is to import the East Texas project. This will read in the MODFLOW model and solution, and all other files associated with the model.

To import the project:

1. Select the *Open* button .
2. Locate and open the directory entitled **tutfiles\modfmap\sample**.
3. Select the file entitled **sample.gpr**.
4. Choose the *Open* button.

7.5 Defining the Units

First, we will define the units. We will not change the length and time units (these must be consistent with the flow model). However, we need to define units for mass and concentration.

1. Select the *Edit | Units* command.
2. Select *slug* for the *Mass* units.
3. Select *ppm* for the *Concentration* units.
4. Select the *OK* button.

7.6 Initializing the MT3DMS Simulation

Now that the MODFLOW model is in memory, we can initialize the MT3DMS simulation. First, we will initialize the model.

1. Switch to the *3D Grid* module .
2. Select the *MT3D | New Simulation* command.

7.6.1 Defining the Species

Since MT3DMS is a multi-species model, we need to define the number of species and name each species. We will use one species named “leachate.”

1. Select the *Define Species* button.
2. Change the name of the species to **leachate**.
3. Select the *OK* button to return to the *Basic Transport Package* dialog.

7.6.2 Defining the Stress Periods

Next, we will define the stress periods.

1. Select the *Stress Periods* button.

Since the flow solution computed by MODFLOW is steady state, we are free to define any sequence of stress periods and time steps we wish. Since the leachate from the landfill will be released at a constant rate, we only need one stress period. We will enter the length of the stress period (i.e., the length of the simulation) and let MT3DMS compute the appropriate transport time step length by leaving the transport step size at zero.

1. Enter **3000** for the stress period length (days).
2. Enter **2000** for the *Max transport steps*.
3. Select the *OK* button to exit the *Stress Periods* dialog.

7.6.3 Selecting Output Control

By default, MT3DMS outputs a solution at every transport step. Since this results in a rather large output file, we will change the output so that a solution is written every time step (every 300 days).

1. Select the *Output Control* button.
2. Select the *Print or save at specified times* option.
3. Select the *Times* button.
4. Select the *Initialize Values* button.

5. Enter the following values:
 - *Initial time step size*: **300**
 - *Bias*: **1**
 - *Maximum time step size*: **300**
 - *Maximum simulation time*: **3000**
6. Select the *OK* or *Close* buttons three times to return to the *Basic Transport Package* dialog.

7.6.4 Selecting the Packages

Next, we will specify which of the MT3DMS packages we intend to use.

1. Select the *Packages* button.
2. Turn on the following packages:
 - *Advection package*
 - *Dispersion package*
 - *Source/Sink Mixing package*
 - *GCG package options*.
3. Select the *OK* button.

Note that the *Basic Transport Package* dialog also includes some layer data. We will address the data for these arrays at a latter point in the tutorial.

4. Select the *OK* button to exit the *Basic Transport Package* dialog.

7.7 Assigning the Aquifer Properties

MT3DMS requires that a porosity and dispersion coefficient be defined for each of the cells in the grid. While these values can be assigned directly to the cells, it is sometimes convenient to assign the parameters using polygonal zones defined in the conceptual model. The parameters are converted to the grid cells using the *Map* → *MT3DMS* command.

7.7.1 Turning on Transport

To assign the porosities and dispersion coefficients to the polygons:

1. Switch to the *Map* module .
2. In the *Data Tree*, right click the **East Texas** conceptual model and select the *Properties* command from the pop-up menu.

3. Turn on *Transport* and make sure **MT3DMS** is selected as the *Transport model*.
4. Click on the *Define Species* button.
5. Click the *New* button to create a new species. Change the species name to **leachate** and click *OK*.
6. Click *OK* to exit the *Conceptual Model Properties* dialog.
7. Expand the **East Texas** conceptual model if necessary to see the coverages under it.
8. In the *Data Tree*, right click the **Layer 1** coverage and select the *Coverage Setup* command from the pop-up menu.
9. In the list of *Areal Properties*, turn on the following:
 - *Porosity*
 - *Long. Dispersivity*
10. Click *OK*.
11. Repeat steps 7 – 9 for the **Layer 2** coverage.

7.7.2 Assigning the Parameters to the Polygons

To assign the porosities and dispersion coefficients to the polygons:

1. Make **Layer 1** the active coverage by selecting it in the *Data Tree*.
2. Choose the *Select Polygons* tool .
3. Double click on the layer polygon.
4. For the *Porosity* enter a value of **0.3**.
5. For *Long. Disp.* enter a value **20**.
6. Select the *OK* button.

To assign the values to layer 2:

1. Make **Layer 2** the active coverage by selecting it in the *Data Tree*.
2. Double click on the layer polygon.
3. For the *Porosity* enter a value of **0.4**.
4. For *Long. Disp.* enter a value **20**.

5. Select the *OK* button.
6. Click anywhere outside the model to unselect the highlighted polygon.

7.8 Assigning the Recharge Concentration

The purpose of our model is to simulate the transport of contaminants emitted from the landfill. When the flow model was constructed, a separate, reduced value of recharge was assigned to the landfill site. This recharge represents leachate from the landfill. We will assign a concentration to this recharge. The concentration can be assigned directly to the recharge polygon in the conceptual model.

1. In the *Data Tree*, right click the **Recharge** coverage and select the *Coverage Setup* command from the pop-up menu.
2. From the list of *Areal Properties*, turn on *Recharge conc.* and click *OK*.
3. Double click on the landfill polygon.
4. For the *leachate Recharge conc.* enter a constant value of **20000** for the concentration.
5. Select the *OK* button.
6. Click anywhere outside the model to unselect the polygon.

7.9 Converting the Conceptual Model

At this point, we are ready to assign the aquifer parameters and the recharge concentration to the cells using the conceptual model.

1. Select the *Feature Objects | Map → MT3DMS* command.
2. Make sure the *All applicable coverages* option is selected and select *OK* at the prompt.

7.10 Layer Thicknesses

To define the aquifer geometry, MT3DMS requires an HTOP array defining the top elevations of the uppermost aquifer. A thickness array must then be entered for each layer. Since we defined the layer geometry in the MODFLOW model, no further input is necessary.

7.11 The Advection Package

Before running MT3D, there are a few more options to enter. First, we need to select a solver for the Advection package. We want to use the *Third Order TVD scheme (ULTIMATE)* solution scheme. This is the default, so we don't need to do anything.

7.12 The Dispersion Package

Next, we will enter the data for the Dispersion package.

1. Switch to the *3D Grid* module .
2. Select the *MT3D | Dispersion Package* command.

The longitudinal dispersivity values were automatically assigned from the conceptual model. All we need to do is specify the remaining three parameters.

3. Enter a value of **0.2** for the *Ratio of transverse dispersivity to longitudinal dispersivity* parameter.
4. Enter a value of **0.2** for the *Ratio of vertical dispersivity to longitudinal dispersivity* parameter.
5. Ensure that the value of the *Effective molecular diff. coefficient* is **0**.
6. Change the *Layer* to **2**.
7. Once again, enter **0.2** for both dispersivity ratios.
8. Select the *OK* button to exit the *Dispersion Package* dialog.

7.13 The Source/Sink Mixing Package Dialog

Finally, we must define the data for the source/sink mixing package. However, the only data required in this package for our simulation are the concentrations assigned to the recharge from the landfill. These values were automatically assigned to the appropriate cells from the conceptual model. Thus, the input data for this package are complete.

7.14 Saving the Simulation

We are now finished inputting the MT3DMS data and we are ready to save the model and run the simulation. To save the simulation:

1. Select the *File | Save As* command.
2. Locate and open the directory entitled **tutfiles\mt3dmap**.
3. Enter **run1.gpr** for the file name.
4. Select the *Save* button to save the files.

7.15 Running MODFLOW

MT3D requires the .hff file generated by MODFLOW. Since we saved the project in a different folder than the one where we opened the MODFLOW simulation from, the .hff file does not exist in the new location. We need to rerun MODFLOW so that it will recreate the .hff file in the current folder.

To run MODFLOW:

1. Select the *MODFLOW | Run MODFLOW* command.
2. Select *OK* at the prompt if it appears.
3. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

7.16 Running MT3DMS

To run MT3DMS:

1. Select the *MT3D | Run MT3DMS* command.
2. Select *Yes* at the prompt to save your changes.
3. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

7.17 Viewing the Solution

1. In the *Time Step* list below the *Data Tree*, select the last time step.

It is often helpful to use the color filled contours option. To do this:

2. Select the *Data | Contour Options* command.
3. Select the *Contour specified range* option.
4. Enter **1** for the minimum value and **125** for the maximum.

5. Change the *Contour Method* to *Color fill*.
6. Select the *OK* button to exit the *Contour Options* dialog.

You should now see a display of color shaded contours confined to the area adjacent to the landfill. Note that the leachate eventually reaches both the river and the well. To view the solution for layer two:

7. Select the down arrow ↓ in the mini-grid display.

To view the solution in cross section view:

8. Select the up arrow ↑ in the mini-grid display.
9. Select a cell in the vicinity of the landfill.
10. Select the *View J Axis* button .
11. Use the left ← and right → arrow keys to view the solution along different columns.
12. Select the *View K Axis* button  when finished.

7.18 Viewing an Animation

Next, we will observe how the solution changes over the course of the simulation by generating an animation. To set up the animation:

1. Select the *Display | Animate* command.
2. Make sure the *Data set* option is on and click *Next*.
3. Turn on the *Display clock* option.
4. Select the *Use constant interval* option.
5. Enter a value of **300** for the *Time interval*.
6. Select the *Finish* button.

You should see some images appear on the screen. These are the frames of the animation which are being generated.

1. After viewing the animation, select the *Stop*  button to stop the animation.
2. Select the *Step*  button to move the animation one frame at a time.

3. You may wish to experiment with some of the other playback controls. When you are finished, close the window and return to GMS.

7.19 Modeling Sorption and Decay

The solution we have just computed can be thought of as a worst case scenario since we have neglected sorption and decay. Sorption will retard the movement of the plume and decay (due to biodegradation) will reduce the concentration. For the second part of the tutorial we will modify the model so that sorption and decay are simulated. We will then compare this solution with the first solution.

7.19.1 Turning on the Chemical Reactions Package

Sorption and decay are simulated in the *Chemical Reactions Package*. We need to turn this package on before it can be used.

1. Select the *MT3D | Basic Transport Package* command.
2. Select the *Packages* command.
3. Turn on the *Chemical reaction package* option.
4. Select the *OK* button to exit the *Packages* dialog.
5. Select the *OK* button to exit the *Basic Transport Package* dialog.

7.19.2 Entering the Sorption and Biodegradation Data

Next, we will enter the sorption and biodegradation data in the *Chemical Reactions Package* dialog.

1. Select the *MT3D | Chemical Reaction Package* command.
2. In the *Sorption* section, select the **Linear isotherm** option.
3. In the *Kinetic rate reaction* section, select the **First-order irreversible kinetic reaction** option.
4. In the lower part of the dialog, enter the following values:

<i>Bulk density</i>	104
<i>1st sorption constant</i>	0.003
<i>Rate constant, dissolved phase</i>	0.0001
<i>Rate constant, sorbed phase</i>	0.0001

5. Switch the layer to layer **2** and enter the following values:

<i>Bulk density</i>	100
<i>1st sorption constant</i>	0.003
<i>Rate constant, dissolved phase</i>	0.00005
<i>Rate constant, sorbed phase</i>	0.00005

6. Select the *OK* button to exit the dialog.

7.20 Run Options

We are about ready to save the project under a new file name. However, we will face the same problem we did earlier with the .hff file. That is, MT3D will look for a .hff file with the same name as the one we are about to use to save the project. That file doesn't exist. We could rerun MODFLOW to create it, but there's another way.

1. Select the *MT3D | Run Options* command.
2. Select the *Single run with selected MODFLOW solution* option. Make sure that **run1 (MODFLOW)** is the selected solution.
3. Select *OK*.

With this option, GMS tells MT3D to use the .hff file we generated previously.

7.21 Saving the Simulation

We are now ready to save the new simulation.

1. Select the *File | Save As* command.
2. Enter **run2.gpr** for the file name.
3. Select the *Save* button.

7.22 Running MT3DMS

To run MT3DMS:

1. Select the *MT3D | Run MT3DMS* command.
2. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

7.23 Viewing the Solution

After the simulation finishes and the solution is read:

1. In the *Time Step* list below the *Data Tree*, select the last time step.

Notice that at the end of the simulation the plume is smaller and less advanced than in the first simulation.

7.24 Generating a Time History Plot

A useful way to compare two transient solutions is to create an observation point and generate a time history plot. The fastest way to do this is to create an “Active Data Set Time Series” plot.

7.24.1 Creating a Time Series Plot

1. Select the *Plot Wizard* button .
2. Select the *Active Data Set Time Series* option for the plot type.
3. Select the *Finish* button.
4. Select a cell in the grid near the landfill. Notice that the plot shows the concentration v. time.
5. Select a different cell and notice that the plot updates. If no cell is selected then the plot will not show any data.

If you want to take the plot data and put it into Excel you can right click on the plot and select the view values option. This brings up a spreadsheet that you can copy and then paste into Excel.

7.25 Conclusion

This concludes the *MT3DMS – Conceptual Model Approach* tutorial. Here are the things that you should have learned in this tutorial:

- If you are starting with a MODFLOW conceptual model, you must turn on transport in the conceptual model properties.
- You can use the *MT3D | Run Options* command to tell MT3D what MODFLOW solution you want to use.

Model Calibration

An important part of any groundwater modeling exercise is the model calibration process. In order for a groundwater model to be used in any type of predictive role, it must be demonstrated that the model can successfully simulate observed aquifer behavior. Calibration is a process wherein certain parameters of the model such as recharge and hydraulic conductivity are altered in a systematic fashion and the model is repeatedly run until the computed solution matches field-observed values within an acceptable level of accuracy. GMS contains a suite of tools to assist in the model calibration process. These tools are described in this tutorial.

The model calibration exercise in this tutorial is based on the MODFLOW model. Thus, you may wish to complete the *MODFLOW - Conceptual Model Approach* tutorial prior to beginning this tutorial. Although this particular exercise is based on MODFLOW, the calibration tools in GMS are designed in a general purpose fashion and can be used with any model.

8.1 Description of Problem

A groundwater model for a medium-sized basin is shown in Figure 8-1. The basin encompasses 28 square miles. It is in a semi-arid climate, with average annual precipitation of 1.25 ft/yr. Most of this precipitation is lost through evapotranspiration. The recharge which reaches the aquifer eventually drains into a small stream at the center of the basin. This stream drains to the north and eventually empties into a lake with elevation 1000 ft. Three wells in the basin also extract water from the aquifer. The perimeter of the basin is bounded by low permeability crystalline rock. There are ten observation wells in the basin. There is also a stream flow gauge at the bottom end of the stream.

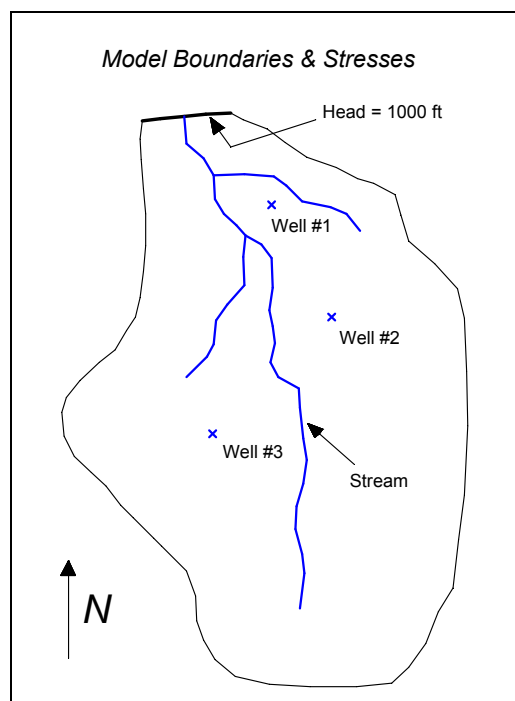


Figure 8-1 Sample Model Used in Calibration Exercise.

The assumed recharge and hydraulic conductivity zones for the model are shown in Figure 8-2. The model region encompasses fractured and weathered bedrock as well as alluvial material, grading from hydraulically tighter materials in the south to more permeable materials in the north. Furthermore, the materials around the stream tend to be coarser, cleaner, and thus more permeable. The topmost region of the model near the lake has a high level of phreatophytic plant life.

The first task of this exercise will be to import a single layer, unconfined MODFLOW model that has been constructed for the site. This model contains an initial estimate of hydraulic conductivities and recharge. A solution computed with this initial model will then be imported and the error in the initial solution will be analyzed. New values for hydraulic conductivity and/or recharge will then be entered, a new solution will be generated, and a new error estimate will be computed. These steps will be repeated until the error is reasonably small.

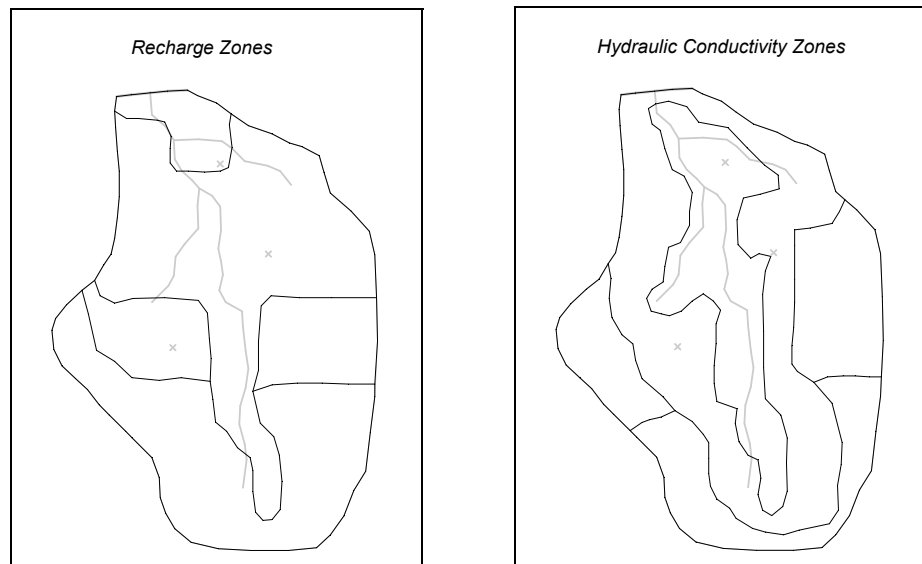


Figure 8-2 Recharge and Hydraulic Conductivity Zones.

8.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

8.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW

You can see if these components are enabled by selecting the *File | Register* command.

8.4 Reading in the Model

First, we will read in the model:

1. Select the *Open* button .
2. Locate and open the **tutfiles\calib** directory.
3. Select the file entitled **bigval.gpr**.

4. Select the *Open* button.

You should see both a grid and a conceptual model appear. The conceptual model consists of three coverages. The currently active coverage contains the model boundary, the specified head boundary, the stream, and the wells. There is also a coverage of recharge zones and a coverage of hydraulic conductivity zones. For the initial simulation, a single value of hydraulic conductivity (8 ft/day) and a single value of recharge ($2.5\text{e-}4$ ft/day) have been assigned. The polygonal zones of hydraulic conductivity and recharge will be edited as the tutorial progresses to reduce the model error.

The conceptual model was used to construct the MODFLOW model that is shown.

8.5 Observation Data

We will be using two types of observation data in the calibration process: water table elevations from observation wells and observed flow rates in the stream. Since the model is in a fairly arid region, we will assume that most of the flow to the stream is from groundwater flow.

8.6 Entering Observation Points

First, we will enter a set of observation points representing the observed head in the ten observation wells in the region. Observation points are created in the *Map* module.

8.6.1 Creating a Coverage With Observation Properties

Before entering observation points, we must first create a coverage with observation properties.

1. Switch to the *Map* module .
2. In the *Data Tree*, right-click on the **BigVal** conceptual model and select the *New Coverage* command from the pop-up menu.
3. Name the new coverage **Observation Wells**.
4. In the list of *Observation Points* properties, turn on *Head*.
5. Change the *3D grid layer option for obs. pts* option to **By layer number**.
6. Select the *OK* button to exit the *Observation Coverage* dialog.

8.6.2 Creating an Observation Point

We are now ready to create an observation point. The first point we will be creating has the following values:

x [ft]	y [ft]	Head [ft]	Interval [ft]	Confidence [%]
14661	32694	999.0	1.5	95

The interval represents the estimated error ($\pm$) in the observed value. The confidence value represents the confidence in the error estimate. The interval can be used as a calibration target. Calibration is achieved when the error is within the estimated error interval (± 1.5 ft in this case) of the observed value. In other words, if the computed head falls between 997.5 - 1000.5, the calibration target is reached for this observation well.

To create the point:

1. Select the *Create Point* tool .
2. Click once anywhere on the model.
3. With the point selected, change the *X* and *Y* values in the *Edit Window* to *X: 14661* and *Y: 32694*.

To assign the properties to the point:

1. With the point still selected, select the *Properties* button .
2. Change the name of the point to **Point #1**.
3. Change the *Type* to **obs. pt.**
4. Enter **999** for the *Obs. Head*.
5. Enter **1.5** for the *Obs. Head Interval*.
6. Enter **95** for the *Obs Head conf(%)*.
7. Select the *OK* button.

8.6.3 Calibration Target

At this point, a calibration target like the one shown in Figure 8-3 typically shows up next to the observation point. In this case, however, the observation measurement model is MODFLOW, and with MODFLOW, things are a bit different. With MODFLOW you must run the simulation and read in the solution before the calibration targets appear. This is because the computed values are output by MODFLOW and are not calculated internally by GMS. So, we will now run MODFLOW and read in the solution.

1. Select the *File | Save As* command.
2. Enter **run2.gpr** for the file name.
3. Select the *Save* button.
4. Switch to the *3D Grid* module .
5. Select the *MODFLOW | Run MODFLOW* command.
6. When MODFLOW is finished running, select the *Close* button.

Note that a calibration target is now drawn next to the point. The components of a calibration target are illustrated in Figure 8-3. The center of the target corresponds to the observed value. The top of the target corresponds to the observed value plus the interval and the bottom corresponds to the observed value minus the interval. The colored bar represents the error. If the bar lies entirely within the target, the color bar is drawn in green. If the bar is outside the target but the error is less than 200%, the bar is drawn in yellow. If the error is greater than 200%, the bar is drawn in red.

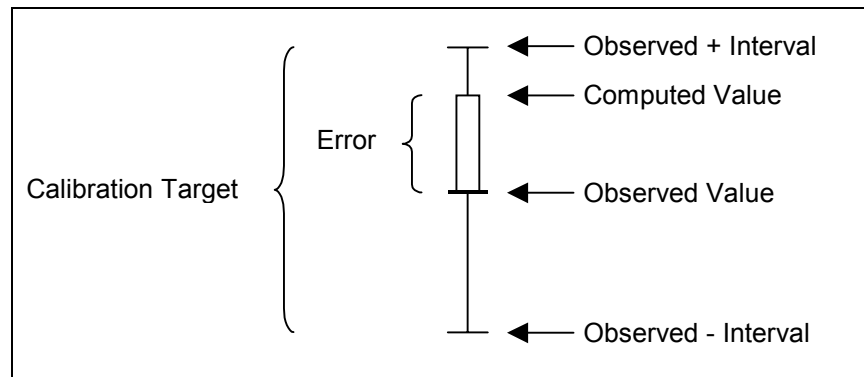


Figure 8-3 Calibration Target.

8.6.4 Point Statistics

We can view more detailed statistics concerning the error at the point by selecting the point.

1. Switch to the *Map* module .
2. Select the *Select Points/Nodes* tool .
3. Click on the observation point.

Notice that a set of statistics related to the point is displayed in the *Help Bar* at the bottom of the GMS screen.

8.7 Reading in a Set of Observation Points

Using the steps defined above, we could proceed to enter the remaining nine observation points. However, in the interest of time, we will simply read in a previously prepared map file containing all ten points.

8.7.1 Deleting the Current Coverage

Before reading in the observation points, we will first delete the current coverage.

1. Select *Observation Wells* coverage in the *Data Tree* and select the *Delete* key.
2. Select the *Delete* command.

8.7.2 Reading in the Points

We will now read in a file containing several observation points.

1. Select the *Open* button .
2. Change the *Files of Type* to ***.map**.
3. Select the file entitled **obswells.map**.
4. Select the *Open* button.

8.8 Entering the Observed Stream Flow

Now that the observation points are defined, we will enter the observed flow in the stream. Observed flows are assigned directly to arcs and polygons in the local source/sink coverage of the conceptual model. We will assign an observed flow to the river arcs. MODFLOW determines the computed flow from the aquifer to the stream. This flow value will be compared to the observed flow.

GMS provides two methods for assigning observed flow: to individual arcs or to a group of arcs. The stream flow that was measured at the site represents the total flow from the aquifer to the stream at the stream outlet at the top of the model. This flow represents the flow from the aquifer to the stream for the entire stream network. Thus, we need to assign the observed flow to a group of arcs. When reading a solution, GMS will then automatically sum the computed flow for all arcs in the group. Before assigning the observed flow, we must first create an arc group:

1. In the *Data Tree*, right-click on the *Sources & Sinks* coverage and select the *Coverage Setup* command.
2. In the list of *Sources/Sinks/BCs*, toggle on the *Observed Flow* row.
3. Select *OK* to exit the dialog.
4. Select the *Select Arcs* tool .
5. While holding down the *Shift* key, click on each of the river arcs.
6. Select the *Feature Object | Create Arc Group* command.

This creates a new object out of the selected objects. We can now assign an observed flow to the arc group.

1. Select the *Select Arc Groups* tool .
2. Double click on any of the river arcs.
3. Turn on the *Obs.flow* option.
4. In the *Obs. flow rate* field, enter a value of **-164000** for the *Flow*.
5. Enter a value of **7500** for the *Obs. Flow int.*.

The values we entered indicate that to achieve calibration, the computed flow should be between -156500 and 171500 ft³/day (164000 +/- 7500).

1. Select the *OK* button to exit the dialog.
2. Click outside the arc group to unselect it.
3. Select the *Save* button .
4. Switch to the *3D Grid* module .
5. Select the *MODFLOW | Run MODFLOW* command.
6. When the model finishes running, select the *Close* button.

At this point, you should see a calibration target appear for the observed flow on the arc group.

8.9 Generating Error Plots

Next, we will generate some plots related to the calibration error. We will create two plots related to error at the observation points.

1. Select the *Plot Wizard* button .
2. Select the *Computed vs. Observed Data* plot.
3. Select the *Next* button.
4. Select the *Finish* button.

In the first plot, a symbol is drawn for each of the observation points. A point that plots on or near the diagonal line indicates a low error. Points far from the diagonal have a larger error.

8.10 Editing the Hydraulic Conductivity

The next step in the calibration exercise is to change the model parameters and re-run the model. Note, if you switch to the observation coverage, that the errors on the left and right side of the model are mostly red and negative. This indicates that the observed value is much larger than the current computed value. We will begin by changing the hydraulic conductivity in these zones. The hydraulic conductivity will be edited by changing the hydraulic conductivity assigned to the polygonal zones in the conceptual model.

Before editing the hydraulic conductivity values, we will first make the hydraulic conductivity zone coverage the active coverage.

1. Switch to the *Map* module .
2. In the *Data Tree*, select the *Hydraulic Conductivity* coverage.

To edit the hydraulic conductivity values:

1. Select the *Select Polygons* tool .
2. While holding the *Shift* key, select polygons 1 and 2 shown in Figure 8-4.
3. Select the *Properties* button .
4. Enter a value of **2** for the *Horizontal K* for each polygon.
5. Select the *OK* button.
6. Double click on polygon 3 shown in Figure 8-4.
7. Enter a value of **0.5** for the *Horizontal K*.
8. Select the *OK* button.

9. Click outside the model to unselect the polygon.

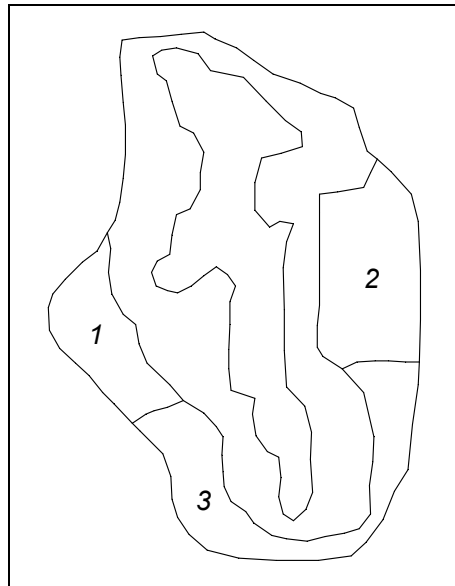


Figure 8-4 Polygons to be Selected.

8.11 Converting the Model

Now that the values have been edited, the next step is to convert the conceptual model to the grid-based numerical model:

1. Select the *Feature Objects | Map → MODFLOW / MODPATH* command from.
2. At the prompt, make sure the *All applicable coverages* option is selected and select *OK*.

8.12 Computing a Solution

The next step is to save the MODFLOW model with the new values and compute a new solution.

8.12.1 Saving the Simulation

To save the simulation:

1. Select the *File | Save As* command.
2. Enter **run3.gpr** for the file name and click *Save*.

8.12.2 Running MODFLOW

To run MODFLOW:

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | Run MODFLOW* command.
3. Select *OK* at the prompt.
4. When the MODFLOW simulation is completed, select the *Close* button. The solution is read in automatically.

Note that the plots in the *Plot Window* have been updated. Up to this point we have not paid much attention to our flow target on the arc group. In the next section, we will create a plot that shows how well the flow target is being met.

Note that although the error improved for the observation wells, the head is still too low on the left and right sides of the model.

8.13 Error vs. Simulation Plot

When performing trial and error calibration, it is important to keep track of the trend in the error as new solutions are repeatedly computed. GMS provides a special calibration plot to simplify this task.

1. Select the *Plot Wizard* button .
2. Select the *Error vs. Simulation* plot.
3. Select the *Next* button.
4. Select the *Finish* button.

The change in each of the three error norms from one solution to the next is clearly visible in the new plot. The plot is updated as each new solution is read in. Ideally, as you make changes to the model, the error should gradually become smaller and smaller. If a bad choice is made in changing the model, the error may temporarily increase. In most cases, it is a good idea to keep a log of the changes made and the resulting errors.

8.14 Continuing the Trial and Error Calibration

At this point, you are free to continue on your own with the trial and error calibration process using the steps outlined above. You may wish to change both the recharge and the hydraulic conductivity values. Before you edit the

recharge values, be sure to make the coverage visible by selecting it in the *Data Tree*.

8.14.1 Changing Values vs. Changing Zones

For this tutorial, you should be able to get a good match between the computed and observed values simply by changing the hydraulic conductivity and recharge values assigned to the polygonal zones. In a real application, however, you may also need to change the size and distribution of the zones, in addition to the values assigned to the zones.

8.14.2 Viewing the Answer

If you wish to view the “answer”, a map file can be imported which contains a set of parameter values which result in a solution that satisfies the calibration target for each of the ten observation wells.

Before reading in the new conceptual model, you must first delete each of the three MODFLOW coverages:

1. Switch to the *Map* module .
2. In the *Data Tree*, highlight and delete each of the three MODFLOW coverages (Sources & Sinks, Recharge, and Hydraulic Conductivity).

To read in the new conceptual model:

1. Select the *Open* button .
2. Select *No* at the prompt to confirm we don't want to save our changes if it appears.
3. Select the file titled **answer.map**.
4. Select the *Open* button.

You can now convert this model to the grid and compute a new solution using the steps described above.

8.15 Conclusion

This concludes the *Model Calibration* tutorial. Here are the things that you should have learned in this tutorial:

- Observation points will display a target next to them that shows how well the computed values match the observed values.

- With MODFLOW, the computed values at the observation points come from MODFLOW and not GMS. Thus, if you create an observation point, you will have to run MODFLOW before you will see a target.
- If you want to specify a flow observation that applies to a network of streams, you can create an arc group.
- A number of different plots are available when doing model calibration.
- Whenever you make changes to the conceptual model you must use the *Feature Objects | Map → MODFLOW / MODPATH* command and save your project before running MODFLOW.

Automated Parameter Estimation

The *Model Calibration* tutorial describes the basic calibration tools provided in GMS. It illustrates how head levels from observation wells and observed flows from streams can be entered into GMS and how these data can be compared to model computed values. It also describes how a trial and error method can be used to iteratively adjust model parameters until the model computed values match the field observed values to an acceptable level of agreement. In many cases, calibration can be achieved much more rapidly with an inverse model. GMS contains an interface to three inverse models: MODFLOW 2000 PES process, PEST, and UCODE. An inverse model is an internal process (MODFLOW 2000 PES process) or an external utility (PEST/UCODE) that automates the parameter estimation process. The inverse model systematically adjusts a user-defined set of input parameters until the difference between the computed and observed values is minimized.

This tutorial illustrates how to calibrate a MODFLOW model using the MODFLOW 2000 PES process and PEST. Since this tutorial assumes you understand how to enter field observed values, you should complete the previous tutorial, *Model Calibration*, prior to beginning this tutorial.

9.1 Description of Problem

The model we will be calibrating in this tutorial is the same model featured in the *Model Calibration* tutorial. The model includes observed flow data for the stream and observed heads at a set of scattered observation wells. The conceptual model for the site consists of a set of recharge and hydraulic conductivity zones. These zones will be marked as parameters and an inverse model will be used to find a set of recharge and hydraulic conductivity values

that minimize the calibration error. We will first use the MODFLOW 2000 PES Process, and then PEST. We will utilize two methods for model parameterization: polygonal zones and pilot point interpolation.

9.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

9.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Geostatistics
- Map
- MODFLOW
- Inverse Modeling

You can see if these components are enabled by selecting the *File | Register* command.

9.4 Reading in the Project

First, we will read in the modeling project:

1. Select the *Open* button .
2. Locate and open the **tutfiles\inverse** directory.
3. Select the file entitled **bigval.gpr**.
4. Select the *Open* button.

You should see a MODFLOW model with a solution and a set of GIS coverages. Three of the coverages are the source/sink, recharge, and hydraulic conductivity coverages used to define the conceptual model. The active coverage contains a set of observed head values from observation wells. If you switch to the source/sink coverage, you will notice that an observed flow has been assigned to the stream network as described in the previous tutorial.

9.5 Model Parameterization

The first step in setting up the inverse model is to “parameterize” the input. This involves identifying which parts of the model input we want the inverse model utility to optimize. We will utilize two approaches for parameterization. In the first attempt at parameter estimation with the MODFLOW 2000 PES Process, we will use the zonal approach. This involves identifying polygonal zones of hydraulic conductivity and recharge, marking the zones as parameters, and assigning a starting value for each zone. The PES Process will then adjust the K or recharge values assigned to the zones as it attempts to minimize the residual error between computed vs. observed heads and flows. In the second part of this tutorial, we will use the pilot point method in conjunction with PEST to parameterize hydraulic conductivity. With the pilot point method, we define a set of scatter points where the hydraulic conductivity is assigned. Each point acts as an independent parameter and the K values for the grid are interpolated from the pilot points. The pilot point method allows for a more continuous, and potentially more complex distribution of values throughout the model domain. It also alleviates the modeler from having to define the distribution of the zones, a process that can be difficult given limited data and is often done in an arbitrary manner.

9.6 Defining the Parameter Zones

For our first attempt at parameter estimation with the MODFLOW 2000 PES Process, we will define a set of parameter zones. The conceptual model approach utilized in GMS is ideally suited for this task since the conceptual model consists of recharge and K zones defined with polygons. We will mark the polygons as parameter zones by assigning a “key value” to each polygon. The key value should be a value that is not expected to occur elsewhere in the MODFLOW input file. A negative value typically works well.

We will use seven parameter zones consisting of four hydraulic conductivity zones and three recharge zones. The number of observations is eleven, consisting of ten observation wells and one stream flow value. Note that the number of parameters being estimated should always be less than the number of observations.

9.6.1 Setting up the Hydraulic Conductivity Zones

First we will set up the hydraulic conductivity zones. The hydraulic conductivity polygons are shown in Figure 9-1. The five polygons will be used to define four parameter zones. The key values associated with each of the four zones are shown on the polygons in the figure.

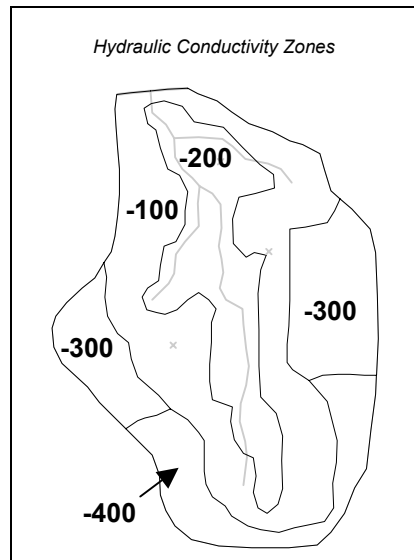


Figure 9-1 Hydraulic Conductivity Zones and Parameter Key Values.

To assign the key values to the polygons:

1. If necessary, switch to the *Map* module .
2. Expand the *Flow Model* conceptual model by clicking the plus symbol next to it in the *Data Tree*.
3. Switch to the *Hydraulic Conductivity* coverage by selecting it from the *Data Tree*.
4. Select the *Select Polygons* tool .
5. Double click on each of the polygons shown in Figure 9-1 and assign the appropriate key value to the *Horizontal K* input field.

9.6.2 Setting up the Recharge Zones

Next, we will set up the recharge zones. The recharge polygons are shown in Figure 8-2. The five polygons will be used to define four parameter zones. The polygon at the top end of the model is relatively small, it is isolated from the majority of the observation wells, and it is downgradient from the wells. As a result, it is not a good candidate for parameter estimation. We will fix the recharge in this zone at zero. The key values will be associated with the other four polygons to define three parameter zones as shown.

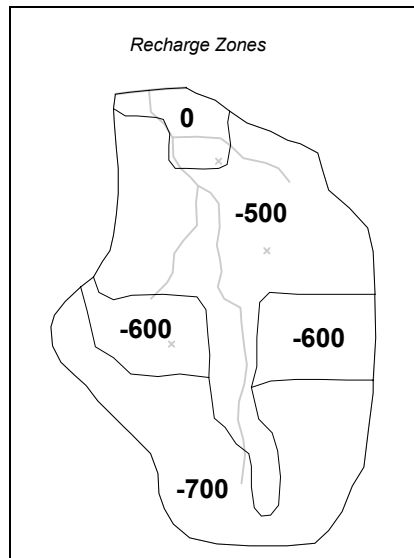


Figure 9-2 Recharge Zones and Parameter Key Values.

To assign the key values to the polygons:

1. Switch to the *Recharge* coverage by selecting it from the *Data Tree*.
2. Double click on each of the polygons shown in Figure 8-2 and assign the appropriate key value to the *Recharge rate* input field.

9.6.3 Mapping the Key Values to the Grid Cells

Once the key values are assigned to the polygons, they must be mapped to the cells in the MODFLOW grid.

1. Select the *Feature Objects | Map → MODFLOW / MODPATH* command.
2. Select *OK* at the prompt.

9.7 Selecting the Parameter Estimation Option

Before we edit the parameter data, we will turn on the *Parameter Estimation* option. This option is turned on in the *Global Options* dialog.

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | Global Options* command.
3. In the *Run Options* section of the dialog select the **Parameter Estimation** option.

4. Select the *Packages* button and select the **MF2K PES Process** in the *Parameter Estimation Engine* section of the packages dialog. Select *OK* to exit the dialog.

9.8 Starting Head

The head contours currently displayed on the grid are from a forward run of a MODFLOW simulation using the starting parameter values. Before running the PES process, we will copy the computed heads to the Starting Heads array. This will ensure that each time PES runs MODFLOW, the starting head values will be reasonably close to the final head values and MODFLOW should converge quickly.

1. Select the *Starting Head* button.
2. Select the *3D Data Set* → *Grid* command.
3. Select the **bigval_HEADS** data set and click *OK*.
4. Select the *OK* button to exit the *Starting Head* dialog.
5. Select the *OK* button to exit the *Global Options* dialog.

9.9 Editing the Parameter Data

Next, we will create a list of parameters and enter a starting, minimum, and maximum value for each.

1. Select the *MODFLOW | Parameters* command.

The *Parameters* section of this dialog is used to manage a list of the parameters used by the inverse model. The *New* button can be used to create a set of parameters one at a time. Each parameter has several properties, including a name, a key value, a type, a starting value, a minimum value, a maximum value, a usage field, and a log-transform field. Rather than creating each parameter one at a time, in most cases the parameter list can be automatically generated by GMS using the *Initialize From Model* button. When this button is selected, GMS searches the MODFLOW input data for likely key values and creates a list of parameters. If a parameter is not automatically found by GMS, it can be added using the *New Parameter* button.

2. Select the *Initialize from Model* button.

Note that all seven parameters were automatically found. Also note that the parameters have been given a default name. The next step is to enter a starting, minimum, and maximum value for each parameter. Special care should be taken when selecting the starting values. In most cases, using arbitrary starting

values will cause the inverse model to fail to converge. The closer the starting values are to the final parameter values, the greater the chance that the inverse model will converge. The starting values we will use were found after a few iterations of manual (trial and error) calibration.

3. Enter the following data into the parameters spreadsheet:

Name	Start Value	Min Value	Max Value
HK_100	4	0.01	100
HK_200	8	0.01	100
HK_300	2	0.01	100
HK_400	0.5	0.01	100
RCH_500	0.00035	1e-10	0.0005
RCH_600	0.00025	1e-10	0.0005
RCH_700	0.00020	1e-10	0.0005

4. For each of the hydraulic conductivity parameters turn on the *Log transform* option.
5. Select *OK* to exit the dialog.

9.10 Max. Iterations

Finally, we will increase the maximum number of iterations used by the solver package. This will increase the likelihood that MODFLOW will converge at each iteration.

1. Select the *MODFLOW | PCG2 Package* command.
2. Change the *Maximum outer iterations* to **100** and the *Maximum inner iterations* to **100**.
3. Select the *OK* button.

9.11 Saving the Project and Running MODFLOW

We are now ready to save the project and run the PES process.

1. Select the *File | Save As* command.
2. Enter **mfpes.gpr** for the file name.
3. Select the *Save* button.
4. Select the *MODFLOW | Run MODFLOW* command.

MODFLOW is now running in Parameter Estimation mode. The spreadsheet in the top-right-hand corner of the dialog shows the error and the parameter values for each iteration of the parameter estimation process. The plot on the left shows the error for each iteration. When MODFLOW is finished running

you can view the optimum parameter values in the spreadsheet. Once the PES process has found the optimum parameter values MODFLOW will run a forward run with the optimum values and output the head solution. This will be the solution that we read in.

Note: If you have room on your screen, you may wish to resize the output window by dragging the handle in the lower right corner of the window.

9.12 Viewing the Solution

Once MODFLOW is done running you can read in the solution.

1. Make sure that the *Read solution on exit* toggle is checked and select the *Close* button.

The contours currently shown on the 3D grid are the heads from the MODFLOW run with the optimum parameter values. We will now look at the observation targets in the map module and the error associated with this model run.

2. Switch to the *Map* module .
3. Select the *Observation Wells* coverage. Notice that the residual error has been greatly reduced for all monitoring wells.
4. Select the *Sources & Sinks* coverage from the *Data Tree*. Notice that the observation target (located near the top of the stream) shows very little residual error.
5. Select the *Select Arc Group* tool .
6. Select the arc group by clicking on a river arc. Notice in the edit strip at the bottom of the graphics window the computed and observed flow is reported.

Next, we will look at some global error norms.

7. Switch back to the *3D Grid* module .
8. Right click on the **mfpes** solution in the *Data Tree* and select the *Properties* command.

This command brings up a spreadsheet showing the residual error (computed – observed) from this model run. The spreadsheet shows the error from the head observations, the flow observations, and the combined weighted observations. You may wish to compare the values from this run to the *bigval* MODFLOW solution.

9. Select the *Done* button to exit the dialog.

To see more information concerning the model run you can look in the *.glo file. If you expand the folder containing the *mfpes* solution you should see a text file in the *Data Tree* named *mfpes.glo*. If you double click on this file it will open in a text editor. This file shows the model inputs as well as information concerning each parameter estimation iteration.

9.13 Loading Optimal Parameter Values

When you are finished using the inverse model it is often desirable to load and view the optimal parameter values. We will now load the optimal parameters.

1. Select the *MODFLOW | Parameters* command.
2. Select the *Import Optimal Values* button.
3. Select the **mfpes._pa** file and select the *Open* button.

Notice that the starting value for all of the parameters has now been changed to the optimal value computed by the inverse model. Since we are now going to use PEST as our inverse model we want the starting values to be the same as we used with the MODFLOW PES process. We will cancel out of this dialog and restore the old starting values.

4. Select the *Cancel* button to exit the dialog.

9.14 PEST

Now we will use PEST as our inverse model to solve the same problem. However, we will use a different method for parameterization. While it certainly is possible to use the zonal method of parameterization with PEST, we would get an answer very similar to the answer the MODFLOW 2000 PES process gave us. However, for this problem we will use the zonal approach for recharge, but we will use the pilot point interpolation method for hydraulic conductivity.

Pilot points can be thought of as a 2D scatter point set. Instead of creating a zone and having the inverse model estimate one value for the entire zone, the value of the parameter within the zone is interpolated from the pilot points. Then the inverse model estimates the values at the pilot points. Figure 9-3 shows a set of pilot points used to estimate horizontal hydraulic conductivity. Notice how the hydraulic conductivity now varies from cell to cell. When the inverse model runs, the values at the pilot points are adjusted and the “surface” defining the variation of K values is warped until the objective function is minimized.

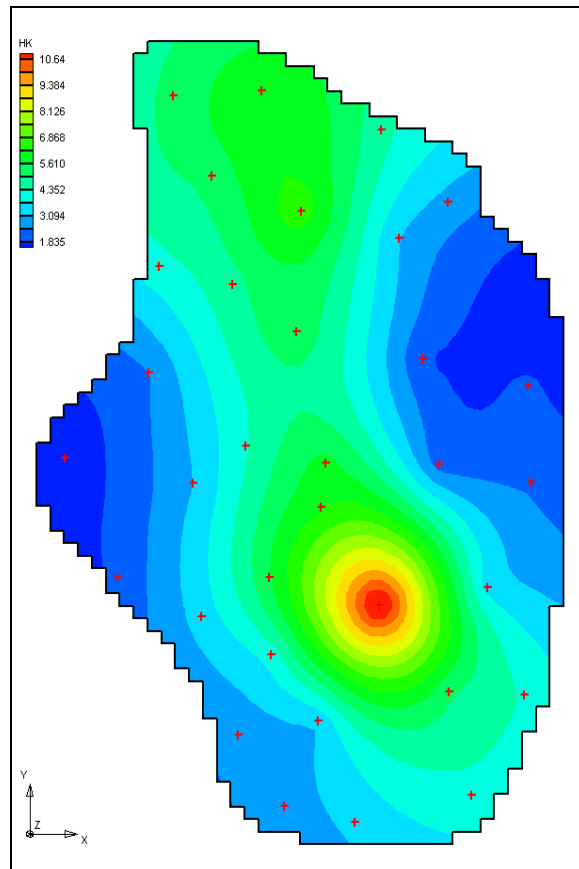


Figure 9-3 Pilot Points and Resulting Conductivity Field

The pilot point method can be used with both the MODFLOW 2000 PES process and PEST. However, PEST provides an additional option for the pilot point method called “regularization”. Regularization imposes an additional measure of “stiffness” to the parameter being interpolated via a “homogeneity” constraint. In the absence of any strong influence from the PEST objective function, this constraint causes values at pilot points to approximate the mean value of adjacent pilot points. This constraint makes the inversion process much more stable and makes it possible to violate one of the typical constraints associated with parameter estimation: namely, the requirement that the number of parameters must be less than the number of observations. With regularization, the number of parameters can greatly exceed the number of observations. As a result, complex hydraulic conductivity distributions can be defined, resulting in extremely low residual error. The pilot point method with regularization is an incredibly powerful feature of PEST.

9.15 Selecting PEST as the Inverse Model

We will now use PEST to calibrate the model.

1. Select the *MODFLOW* | *Global Options* command.

2. Select the *Packages* button.
3. In the *Parameter Estimation Engine* section of the dialog under the, select **PEST**.
4. Select *OK* twice to exit both dialogs.

9.16 Creating Pilot Points

Next, we will create the pilot points that define the hydraulic conductivity distribution for our model. The pilot points are defined as 2D scatter point sets in GMS. We will create about 15 points. In a normal case, we may use 50 or more points. However, additional points slow down the calibration process and 15 points are adequate to illustrate the process with this particular model.

1. Switch to the *2D Scatter Point* module .
2. Select the *Scatter Points | New Scatter Point Set* command.
3. Enter **HK** as the name and select the *OK* button.
4. Select the *Scatter Points | Scatter Point Set Options* command.
5. Enter **5** for the *Default data set value* and select the *OK* button.
6. Select the *Create Vertex* tool .

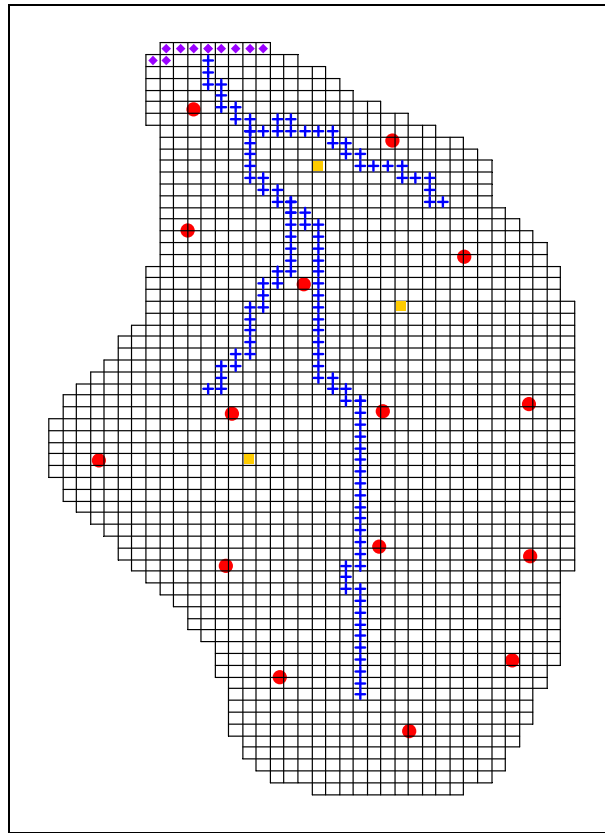


Figure 9-4 Placement of TIN Vertices

7. Click out a set of scatter points similar to those shown in Figure 9-4. Create about 15 points. Don't worry about the exact location of the points, as long as they are distributed in a reasonable fashion.

9.17 Entering the HK parameter

In our previous example we had four hydraulic conductivity parameters. For this problem we are estimating the hydraulic conductivity for the entire layer with pilot points. Therefore, we only need one parameter for hydraulic conductivity. This parameter will then be linked to the pilot points using the *Parameters* dialog.

9.17.1 Creating One Parameter Zone

We will change the values that we have assigned to the polygons so that there is only one hydraulic conductivity parameter.

1. Switch to the *Map* module .
2. Select the **Hydraulic Conductivity** coverage from the *Data Tree*.

3. Select the *Select Polygon* tool .
4. Double click on each of the polygons in the coverage and change the value of the *Horizontal K* input field to **-100**.
5. Select the *Feature Objects | Map → MODFLOW / MODPATH* command to convert the conceptual model.
6. Select *OK* at the prompt.

9.17.2 Editing the Parameters

Now we will edit the parameters that we currently have defined for MODFLOW.

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | Parameters* command.
3. Select the *HK_200* parameter by clicking on the column labeled *HK_200*.
4. Select the *Delete* button.
5. Repeat this process for the *HK_300* and *HK_400* parameters.
6. Turn on the *Pilot Points* option for parameter *HK_100*. Click on the *Options* button in the *Pilot Point Options* column. This brings up the interpolation options dialog. Here you can select the scatter point set and data set used with your parameter as well as the interpolation scheme.
7. The defaults are appropriate in this case so we won't change anything. Select the *OK* button twice to exit the dialogs.

9.17.3 Limiting the Number of Parameter Estimation Runs

In the interest of time we will limit the number of iterations that PEST does for our problem

1. Select the *MODFLOW | Parameter Estimation* command.
2. Change the *Max # of iterations* to **10**.
3. Select *OK* to exit the dialog.

9.18 Saving the Project and Running PEST

We are now ready to save and run PEST.

1. Select the *File | Save As* command.
2. Enter **pest.gpr** for the file name.
3. Select the *Save* button.
4. From the *MODFLOW | Run MODFLOW* command.

PEST is now running. This dialog is similar to the one used when MODFLOW is running in Parameter Estimation mode. The error and parameter values are shown in the spreadsheet in the upper right side of the dialog and the plot on the left shows the error. In this case you may notice some strange parameter names like *sc1v1*. These names were automatically generated and assigned to the scatter points.

PEST will take several minutes to run. You should see the residual error go to an extremely small value. When PEST is finished, you will see a message in the text portion of the window and the *Abort* button will change to *Close*.

9.19 Viewing the Solution

Once PEST is finished, you can read in the solution.

1. Select the *Close* button. Make sure that the *Read solution on exit* toggle is checked.

The contours currently shown on the 3D grid are the heads from the MODFLOW run with the optimum parameter values. We will now look at the observation targets in the map model and the error associated with this model run.

2. Switch to the *Map* module .
3. Select the *Sources & Sinks* coverage from the *Data Tree*. Notice that the observation target on the arc group almost exactly matches.
4. Select the *Select Arc Group* tool .
5. Select the arc group by clicking on the river arc. Notice in the edit strip at the bottom of the graphics window the computed and observed flow is reported.
6. Select the *Observation Wells* coverage from the *Data Tree*. Notice that there is no visible error at any of the observation points.

7. Switch back to the *3D Grid* module .
8. Right click on the *pest* solution in the *Data Tree* and select the *Properties* command.

This command brings up a spreadsheet showing the error from this model run. The spreadsheet shows the error from the head observations, the flow observations, and the combined weighted observations. Note that these values are significantly lower than the values we obtained with the MODFLOW 2000 PES process.

9.20 Viewing the Final Hydraulic Conductivity

When PEST ran a new conductivity value was estimated at each of the scatter points used with the **HK_100** parameter. Now we will read in the optimal parameter values as determined by PEST. Reading in the optimal parameter values will create a new data set for our scatter point set. Then we can interpolate from the scatter point set to the grid to see our final hydraulic conductivity field.

1. Select the *MODFLOW | Parameters* command.
2. Click the *Import Optimal Values* button.
3. Select the **pest.par** file and select the *Open* button. Notice that the starting values for the parameters have changed.
4. Select the *Options* button in the *Pilot Point Options* column for the **HK_100** parameter. Notice that the data set has been changed to **HK_100 (PEST)**.
5. Select *OK* twice to exit the both dialogs.
6. Switch to the *2D Scatter Point* module .
7. Double click on the **HK** scatter point set in the *Data Tree*. You should see 2 data sets below the scatter point set. Make sure that the **HK_100 (PEST)** data set is active.

In order to view the hydraulic conductivity field we need to make sure that the interpolation scheme is the same as the interpolation scheme used for the pilot points.

1. Select the *Interpolation | Interpolation Options* command and make sure that the selected interpolation scheme is *Inverse distance weighted*.

2. Select the *Options* button next to the *Inverse distance weighted* option. Make sure that the nodal function is *Constant*.
3. Select *OK* twice to exit both dialogs.
4. Select the *Interpolation | Interpolate → 3D Grid* command.
5. Select *OK* to accept the default data set name and perform the interpolation.
6. Switch to the *3D Grid module* .
7. Select the *Display | Display Options* command.
8. Turn off the *Contours* option and turn on the *Cell faces* option. Make sure the **Data** colors option is selected below the *Cell faces* option.
9. Select the *Options* button below the *Cell faces* option.
10. In the bottom left portion of the dialog turn on the *Show legend* option.
11. Select *OK* twice to exit both dialogs.

You should now see the final hydraulic conductivity values for you MODFLOW simulation.

9.21 Conclusion

This concludes the *Automated Parameter Estimation* tutorial. Here are the things that you should have learned in this tutorial:

- You can use the zonal approach or the pilot point approach with both PEST and the MF2K PES process, but only PEST includes regularization, thus allowing you to have more pilot points.
- When PEST or MF2K PES finishes, the solution imported into GMS corresponds to the optimal input values. However, the input values in GMS are still the starting values. You must use the *Import Optimal Values* button to replace the starting values with the optimal values.
- You use 2D scatter points to create pilot points in GMS.
- When you are using pilot points and you select the *Import Optimal Values* button, a new data set is created for the 2D scatter points. You then need to interpolate from the scatter points to the grid if you want to see what the array of optimal values is.

Regional to Local Model Conversion

For many modeling studies, determining an appropriate set of boundary conditions can be difficult. It is often the case that classical boundaries such as rock outcroppings, rivers, lakes, and groundwater divides, may be located at a great distance from the site of interest. In such cases, it is often convenient to perform the modeling study in two phases. In the first phase, a large, regional scale model is constructed and the model is extended to well-defined boundaries. During the second stage, a second, smaller, local scale model is constructed that occupies a small area within the regional model. The groundwater elevations computed from the regional model are applied as specified head boundary conditions to the local scale model. The layer data, including elevations and transmissivities, are also interpolated from the regional to the local model. A more detailed representation of the local flow conditions, including low capacity wells and barriers not included in the regional flow model can be constructed in the local scale model. Regional to local model conversion is often referred to as “telescopic grid refinement.”

GMS provides a convenient set of tools that can be used for regional to local model conversion. The steps involved in a typical regional to local model conversion using MODFLOW are described in this tutorial.

10.1 Description of Problem

The site we will be modeling in this tutorial is shown in Figure 10-1. The main features of the regional model are shown. Most of the boundaries are no-flow boundaries corresponding to groundwater flow divides, bedrock outcroppings, and natural flow boundaries. A river runs through the left side of the model. The narrow regions where the river enters and exits the model are modeled as

specified head boundaries. There are four major production wells in the region. The site will be modeled using two layers: a lower confined layer and an upper unconfined layer.

The local site is situated in the interior of the model. The local site corresponds to a chemical plant with a small spill. Once the regional model is completed, a local scale model is to be developed and then used to analyze a number of injection/extraction well placement scenarios. The wells are part of a treatment system that is being designed.

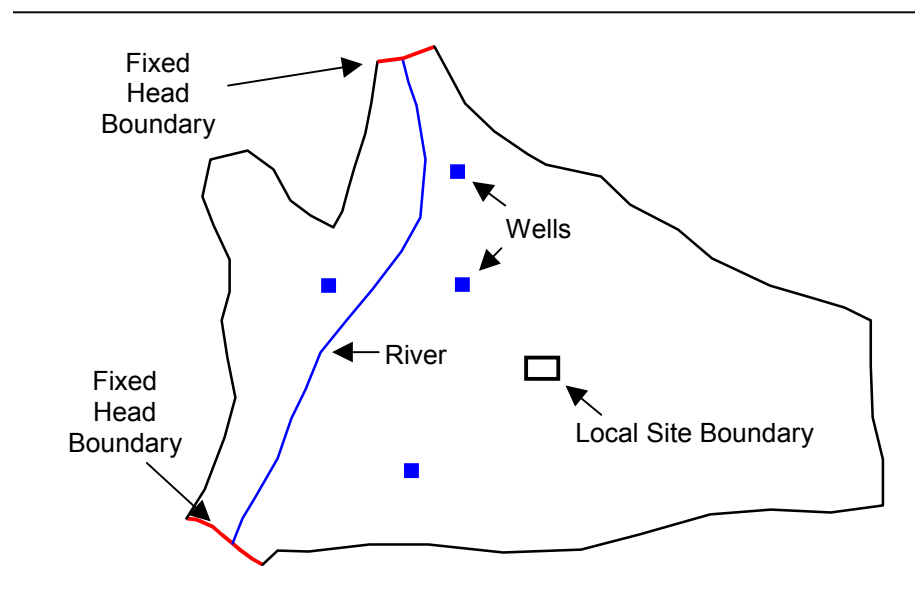


Figure 10-1 Regional Model.

The basic goal of the regional to local model conversion process is to create a 2D scatter point set containing the heads and layer data arrays from the regional model, create the local model, and interpolate the heads and layer data to the local model. A 2D scatter point set is used since the MODFLOW arrays should be interpolated on a layer by layer basis using 2D interpolation. GMS provides a set of tools that greatly simplify this process. The basic steps are as follows:

1. Generate the regional model and compute a solution.
2. Use the *MODFLOW Layers* → *2D Scatter Points* command to create the scatter point set with the layer and head data from the regional model.
3. Create the 3D grid for the local scale model.
4. Interpolate the heads and layer data values from the scatter points to the MODFLOW layer arrays for the local scale model.

Each of these steps will be described in more detail below.

10.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

10.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Geostatistics
- Map
- MODFLOW

You can see if these components are enabled by selecting the *File | Register* command.

10.4 Reading in the Regional Model

The first step in the model conversion process is to build a regional model. Since the focus of this tutorial is primarily on the conversion process, we will read in a previously constructed model.

1. Select the *Open* button .
2. Locate and open the file entitled **tutfiles\reg2loc\regmod.gpr**.

We are now viewing the top layer of the two layer model. You may wish to use the arrow buttons in the *Tool Palette* to view the bottom layer. The wells are located in the bottom layer. When you are finished, return to the top layer.

This model was constructed using the conceptual model approach. The boundary of the local site is indicated with a red rectangle. The conceptual model consists of three coverages. The coverage we are viewing is for the sources and sinks. There is also a coverage defining recharge zones and a coverage defining hydraulic conductivity zones for the top layer. The large rectangular boundary is the grid frame.

The project we imported includes the solution for the regional model. You should see contours of computed head.

10.5 Converting the Layer Data to a Scatter Point Set

The first step in converting the regional model to a local model is to convert the MODFLOW layer data to a 2D scatter point set.

1. Switch to the *3D Grid* module .
2. Select the *Grid | MODFLOW Layers → 2D Scatter Points* command.
3. Change the scatter point set name to *Regional Data*.
4. Select the *OK* button.

You should see a set of scatter points appear at the location of the cell centroids. This scatter point set has a data set for the computed heads and for the top and bottom elevations of the model layers.

10.6 Approach to Building the Local Model

Next, we will build the local model. There are numerous approaches to building the local model. A common approach is to mark the boundaries of the local model as specified head boundaries using the computed head values from the regional model. The following method accomplishes this objective:

A rectangular grid is constructed where two opposite boundaries are parallel to head contours from the regional model (i.e., a constant head value along each boundary). The other two boundaries are no flow boundaries and are perpendicular to the head contours from the regional model.

10.7 Building the Local Conceptual Model

The simplest way to build the local model is to create a conceptual model in the *Map* module. To do this, we will create a new conceptual model.

1. Switch to the *Map* module .
2. Right click on the **Regional Model** item and select the *Duplicate* command.
3. Change the name to **Local Model**.

10.7.1 Creating a New Coverage

Next, we will create a new source/sink coverage.

1. Expand the **Local Model** item in the *Data Tree* by clicking on the plus symbol next to the item.
2. Right-click on the **Copy of ss** coverage and select the *Delete* command from the menu.
3. Right-click on *Local Model* item in the *Data Tree* and select the *New Coverage* command.
4. Change the name of the coverage to **local ss**.
5. In the *Sources/Sinks/BCs* spread sheet toggle on **Specified Head**.
6. Change the *Default layer range* to be **1** to **2**.
7. Select the *OK* button.

Note that we did not delete the recharge and hydraulic conductivity coverages. We will use these coverages to construct our local model. The boundaries of the coverages are larger than they need to be but that does not matter.

10.7.2 Creating the Boundary Arcs

Next, we will create the boundary arcs. First, we need to zoom in on the local site model:

1. Select the *Zoom* tool .
2. Drag a box around the local site boundary (the red rectangle).
3. Select the **local ss** coverage in the *Data Tree* to make it the active coverage.

Create the boundaries as follows:

1. Select the *Create Arc* tool .
2. Create four arcs, two parallel to the contours, and two perpendicular to the contours as shown in Figure 10-2. Double click on the corners to end each arc.

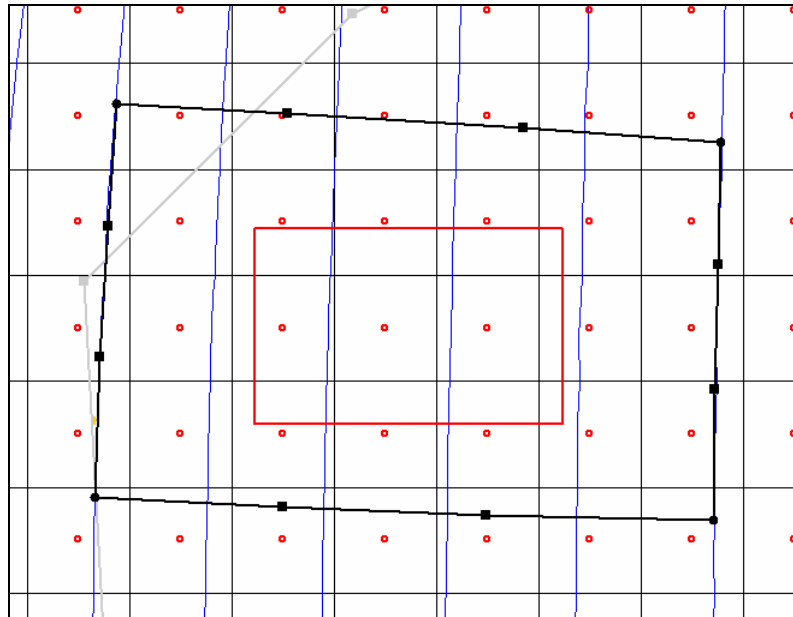


Figure 10-2 Arcs to be Created on Boundary of Local Model.

10.7.3 Building the Polygon

Next, we will use the arcs to build a polygon defining the model domain.

1. Select the *Feature Objects* | *Build Polygons* command.

10.7.4 Marking the Specified Head Arcs

The next step is to mark the specified head boundaries.

1. Select the *Select Arcs* tool .
2. While holding the *Shift* key, select the arcs on the left and right sides of the model.
3. Select *Properties* button .
4. In the *All* row of the spreadsheet change the type to **spec. head**. This will make both arcs specified head arcs.
5. Change the layer assignment so that it goes from **1** to **2**.
6. Select the *OK* button.

At this point we need to select the nodes of the specified head arcs and assign a head value.

1. Select the *Select Points/Nodes* tool .
2. Select the two nodes on the left side of the model.
3. Select *Properties* button .
4. In the Head-Stage field enter a head value of **1050** for both nodes and hit the OK button.
5. Repeat this process for the two nodes on the right side of the model, but assign a head value of **1100**.

10.8 Creating the Local MODFLOW Model

We are now ready to convert the conceptual model to a grid model. First, we will create a new grid frame that fits the local model.

1. Select the *Feature Objects | Grid Frame* command.
2. Select the *OK* at the prompt.
3. If desired, you can use grid frame tool  to position the grid frame to better match the local grid boundary.

10.8.1 Creating the Grid

Next, we will create the grid.

1. Select the *Feature Objects | Map → 3D Grid* command.
2. Select *OK* to confirm the deletion of the current 3D grid.
3. Select *OK* again to confirm deletion of the MODFLOW data.
4. In the *Create Grid* dialog, enter **60** for the number of cells in the x direction, **50** for the number of cells in the y direction, and **2** for the number of cells in the z direction.
5. Select *OK* to create the grid.

You should see a grid appear. You can zoom in to examine the grid.

1. Select the *Zoom* tool .
2. Drag a box around the grid.

10.8.2 Activating the Cells

Next, we will inactivate the exterior cells.

1. Select the *Activate Cells in Coverage* command from the *Feature Objects* menu. If the arcs match the grid boundary closely, you may not see any cells inactivated. If, however, the grid extends significantly beyond the arcs, some cells will be inactivated.

10.8.3 Mapping the Properties

Next, we will convert the MODFLOW data to the grid.

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | New Simulation* command.
3. Select *OK* to accept the defaults in the *MODFLOW Global / Basic Package* dialog.
4. Switch back to the *Map* module .
5. In the *Feature Object | Map* → *MODFLOW / MODPATH* command.
6. Select *OK* at the prompt.

Note: At this point, our local scale model does not include the wells involved in the pump and treat system. These could be added at a later time.

10.9 Interpolating the Layer Data

The final step in the conversion process is to interpolate the regional data from the scatter points to the MODFLOW layer arrays.

1. Switch to the *2D Scatter Point* module .
2. Select the *Interpolation | to MODFLOW Layers* command.
3. Select the *OK* button.

Now that we're done using the scatter points, let's turn them off to make it easier to see the grid.

4. Uncheck the box in the *Data Tree* next to the *2D Scatter Data* folder.

10.10 Saving and Running the Local Model

We are now ready to save the MODFLOW model and run the simulation.

1. Switch to the *3D Grid* module .
2. Select the *File | Save As* command.
3. Change the filename to **locmod.gpr**.
4. Select the *Save* button.

To run MODFLOW:

1. Select the *MODFLOW | Run MODFLOW* command.
2. Select *OK* at the prompt.
3. When the simulation is finished, select the *Close* button.

You should see a set of head contours that closely resemble the head contours from the regional model. At this point, the local flow model is complete and the injection and extraction wells could be added for the pump and treat simulations.

10.11 Conclusion

This concludes the *Regional to Local Model Conversion* tutorial. Here are the things that you should have learned in this tutorial:

- The *Grid | MODFLOW Layers → 2D Scatter Points* command converts your MODFLOW elevation data into scatter points.
- The basic steps for doing Regional to Local model conversion in GMS are:
 1. Generate the regional model and compute a solution.
 2. Use the *MODFLOW Layers → 2D Scatter Points* command to create the scatter point set with the layer and head data from the regional model.
 3. Create the 3D grid for the local scale model.
 4. Interpolate the heads and layer data values from the scatter points to the MODFLOW layer arrays for the local scale model.

Managing Transient Data

Building a transient simulation typically requires the management of large amounts of transient data from a variety of sources including pumping well data, recharge data, river stages, and water levels in observation wells. Gathering and formatting such data can be very tedious. Fortunately, GMS provides a powerful suite of tools for inputting and managing transient data. These tools allow all data to be managed using a date/time format that eliminates much of the extra data processing that is often required with modeling projects. This tutorial illustrates how these tools are used.

This tutorial is based on the MODFLOW model. It is recommended that you complete the *MODFLOW - Conceptual Model Approach* tutorial prior to beginning this tutorial. Although, this particular model is based on MODFLOW, the tools associated with transient data are designed as general-purpose tools and can be used with other models.

11.1 Description of Problem

The model we will be using in this tutorial is the same model used in the *Model Calibration* tutorial. We will use the computed heads from the steady-state calibrated flow model as the starting heads for our transient simulation. Transient recharge and pumping conditions will be modeled. The recharge rates will be manually entered but the pumping rates will be imported from a text file. We will also import a set of transient-field-observed heads from observation wells.

11.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

11.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW

You can see if these components are enabled by selecting the *File | Register* command.

11.4 Reading in the Project

First, we will read in the project:

1. Select the *Open* button .
2. Locate and open the **tutfiles\trans** directory.
3. Select the file entitled **start.gpr**.
4. Select the *Open* button.

You should see a MODFLOW model with a solution and a set of GIS coverages. Two of the coverages are the source/sink and hydraulic conductivity coverages used to define the conceptual model. The active coverage is the recharge coverage.

11.5 Transient Data Strategy

When entering the time values associated with transient data, MODFLOW requires that the time be entered as scalar time values relative to a time value of zero at the beginning of the simulation. Furthermore, the times must be compatible with the time unit selected for the model. This approach can be time-consuming since transient data must be converted from a date/time format to relative time format. The strategy used in GMS for managing transient data makes it possible to enter all time values using a simple date/time format. Transient data are entered in the conceptual model using date/time values. The time at the beginning of the first MODFLOW stress period is the reference time. This represents the date/time corresponding to $t=0$ in the simulation.

When the model is converted from the conceptual model to the grid model, the time values in the conceptual model are automatically mapped to the appropriate time values corresponding to the MODFLOW stress periods. When the MODFLOW model is saved to disk, the date/time values are converted to the appropriate relative time values.

In addition to ease of use, another advantage of the transient data strategy used in GMS is that both the spatial and temporal components of the conceptual model are defined independently of the discretization used in both the grid spacing and the stress period size. The user can change the stress period spacing and regenerate the model from the conceptual model in seconds.

11.6 Entering Transient Data in the Map Module

The first step in setting up our transient model is to associate our transient data with the feature objects in the Map Module.

11.6.1 Assigning the Transient Recharge Rate

First, we will assign the transient recharge rate for the recharge zones. The recharge zones are shown in Figure 11-1. There are four recharge zones defined by five polygons. We will leave the recharge rate for zone 1 at zero. We will assign a transient recharge rate to the other three zones.

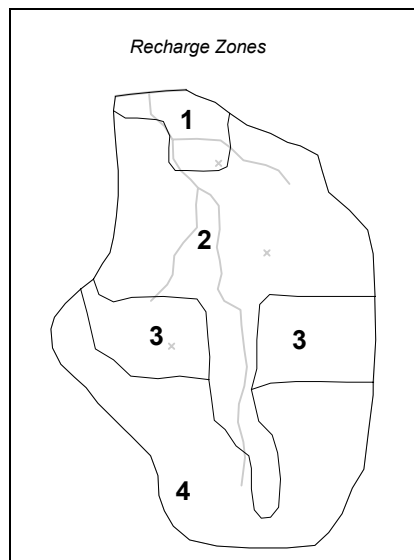


Figure 11-1 Recharge Zones

To assign the recharge data:

1. Switch to the *Map* module .

2. Expand the **Conceptual Model** item in the *Data Tree*.
3. Select the **Recharge** coverage to make it active.
4. Choose the *Select Polygon* tool .
5. Select the polygon corresponding to recharge zone 2 in Figure 11-1.
6. Select *Properties* button .
7. For the *Recharge rate*, click the down arrow  button and select the **<transient>** option from the drop down list.
8. Now click the  button for the *Recharge rate* to bring up the *XY Series Editor*.
9. Select the *Use dates/times* toggle.
10. Enter the following date/times and recharge rates:

Date/Time	Recharge Rate (ft/day)
10/1/1985 12:00:00 AM	0.001
1/1/1986 12:00:00 AM	0.001
1/1/1986 12:00:00 AM	0.0005
3/1/1986 12:00:00 AM	0.0005
3/1/1986 12:00:00 AM	0.006
7/1/1986 12:00:00 AM	0.006
7/1/1986 12:00:00 AM	0.005
10/1/1986 12:00:00 AM	0.005
10/1/1986 12:00:00 AM	0.001
12/1/1986 12:00:00 AM	0.001

11. Select the *OK* button twice to exit both dialogs.

Instead of repeating this same procedure for the other recharge zones we will import previously generated time series curves. These curves were generated using this same editor and saved to text files using the *Export* button.

1. Select the two polygons that make up recharge zone 3 in Figure 11-1. Click on the first polygon and then hold down the *Shift* key while clicking on the second polygon.
2. Select *Properties* button .
3. In the *Recharge Rate* column for the first polygon, select the down arrow  button and select the **<transient>** option from the drop down list.
4. Now click the  button for the *Recharge rate* to bring up the *XY Series Editor*.
5. Select the *Import* button on the right side of the dialog.

6. Select the file named **zone3.xys**.
7. Select the *Open* button. A time series curve should appear in the dialog. Click *OK*.
8. Repeat steps 3-7 for the other polygon.
9. Select the *OK* button.
10. Repeat the same procedure with recharge zone 4 except import the file named *zone4.xys*.

11.6.2 Importing Pumping Well Data

In addition to the transient recharge data, our simulation will also contain a transient pumping schedule for the three wells in the model. Since our model only has three wells, the transient pumping schedules could easily be entered by hand. However, we will import the well data from a text file. This method is particularly useful for models with lots of wells and/or complicated pumping schedules.

Pumping well data is typically imported using two files. The first file contains the name, screen geometry, and xy coordinates of the wells. The second file contains the pumping schedules. Since the well locations are already defined, we only need to import the pumping schedules. The format for this file is as follows:

Name	date	time	Q
"well 1"	12/3/1999	18:00:00	625.0
"well 1"	1/30/2000	7:38:25	0.0
"well 1"	3/27/2000	18:00:00	200.0
"well 2"	12/3/1999	18:00:00	0.0
"well 2"	12/5/1999	14:48:32	100.0
...			

The name column must be included. This tells GMS how to link the transient pumping data to the wells in the map module. The first time an entry is found for a particular well, if the well is steady state, it is changed to transient and a pumping rate time series is created for the well. Each time a subsequent line is read with the same well name, GMS adds a point to the time series. The dates and times can be in any standard format.

To import the well pumping data file:

1. Select the **Sources & Sinks** coverage from the *Data Tree* to make it the active coverage.
2. Select the *Open* button .
3. In the *Open* dialog, change the *Files of type* selection to **Text Files (*.txt)**.

4. Select the file named **pumping.txt** and click *Open*.
5. In the *Import Wizard*, turn on the *Heading row* option and click *Next*.
6. Change the *GMS data type* to **Pumping data** and click *Finish*.
7. Select *Yes* at the prompt to import the pumping data as a step function.
8. Select the *Select Points/Nodes* tool .
9. Double-click on any of the wells and note that the *Flow rate* says **<transient>**. You may want to click on the  button to see the curve.
10. Select *OK* to exit the dialog(s).

11.6.3 Assigning Specific Yield

Next, we need to assign the storage coefficient to the aquifer. Since this is a 1 layer unconfined aquifer, we need to assign the specific yield.

1. Double click on the **Hydraulic Conductivity** coverage in the *Data Tree* to bring up the *Coverage Setup* dialog.
2. In the list of *Areal Properties*, turn on *Specific yield*.
3. Click *OK* to exit the dialog.
4. Select the *Select Polygon* tool .
5. Select the polygons labeled 1 and 2 in the figure below.

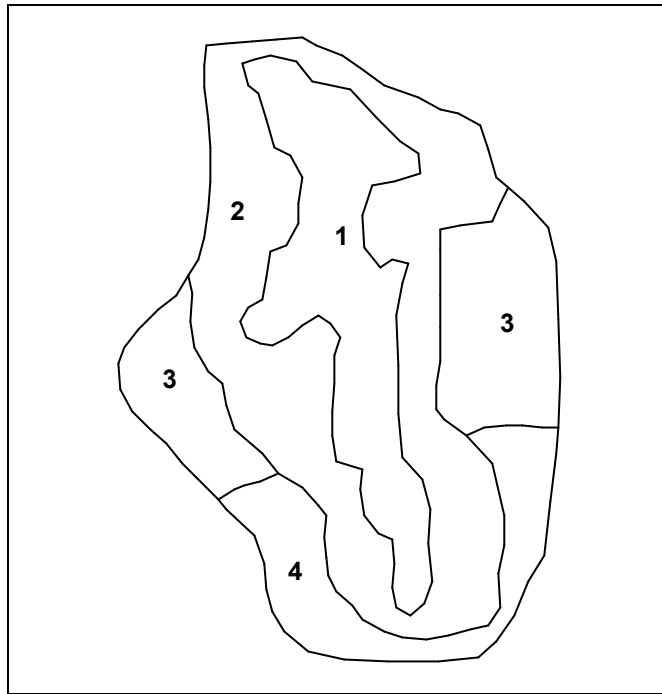


Figure 11-2 Hydraulic Conductivity Zones

6. Select *Properties* button .
7. Assign a *Specific yield* value of **0.20** to both polygons and select the *OK* button to exit the dialog.
8. Repeat the same procedure with the polygons labeled 3 and 4 only this time assign a value of **0.15** for the specific yield.

11.7 Initializing MODFLOW Stress Periods

Before converting our conceptual model we need to set up the stress periods.

11.7.1 Changing the MODFLOW Simulation to Transient

First, we will change the current MODFLOW simulation from a steady-state simulation to transient.

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | Global Options* command.
3. Select the *Transient* option.

11.7.2 Setting up the Stress Periods

Now we will set up the stress period information for MODFLOW.

1. Select the *Stress Periods* button.
2. Turn on the *Use dates/times* option.

When the *Use dates/times* option is used, all input fields in the MODFLOW interface in the *3D Grid* module expect the date/time format for input. The date/time format is used to display time values such as the time step values when post-processing. If the option is not used, scalar time values (e.g., 100, 120, etc.) are displayed.

3. Change the *Number of stress periods* to 7.

We want the stress periods to match the times where our input data in the map module changes. For example, the value for recharge changes at three different dates 1/1/1986, 3/1/1986, and 7/1/1986. Therefore, we need to make sure that we have stress periods that start at those times and at the time corresponding to changes in the pumping schedules.

4. Enter the following times and time steps for the stress periods.

	Start	Num time steps
1	10/1/1985 12:00:00 AM	2
2	1/1/1986 12:00:00 AM	1
3	3/1/1986 12:00:00 AM	8
4	5/1/1986 12:00:00 AM	4
5	6/1/1986 12:00:00 AM	4
6	7/1/1986 12:00:00 AM	8
7	9/1/1986 12:00:00 AM	8
End	12/1/1986 12:00:00 AM	

5. Select the *OK* button to exit the *Stress Periods* dialog.
6. Select the *OK* button to exit the *Global Package* dialog.

11.8 Converting the Conceptual Model

Now we will convert our conceptual model data to MODFLOW input data.

1. Switch to the *Map* module .
2. Select the *Feature Objects | Map → MODFLOW / MODPATH* command.
3. Select *OK* at the prompt.

11.9 Setting Starting Heads

For transient models, you should either set the starting heads equal to the solution generated from a steady state model, or allow some time in the beginning of the transient model for the heads to stabilize before applying any changes in stresses (pumping rates, recharge rates etc.). We'll take the first approach.

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | Global Options* command.
3. Click the *Starting Heads* button.
4. Click the *3D Data Set → Grid* button.
5. In the solution tree, expand the **start (MODFLOW)** solution and select the **start_Heads** data set.
6. Click *OK*.
7. Click *OK* twice more to exit all dialogs.

11.10 Saving and Running MODFLOW

We are now ready to save the model and launch MODFLOW.

1. Select the *File | Save As* command.
2. Enter **trans1.gpr** for the file name.
3. Make sure the *Save simulations in project folder using project filename* option is on.
4. Select the *Save* button.
5. Select the *MODFLOW | Run MODFLOW* command.
6. Once MODFLOW has finished, select the *Close* button to close the window and return to GMS.

The contours should change. Use the *Time Steps* window to cycle through the different time steps of the solution to see how the pumping schedules of the wells affect the computed heads.

11.11 Transient Observation Data

Next, we will input transient observation data for this simulation. Transient observation well data are also entered using the date/time format. The data can be entered either manually or by importing a text file containing the transient measurements. We will use the text file option. We will import the observation point locations from a map file and then import the transient observations from a text file.

11.11.1 Importing Transient Observation Data

First we need to read in the Map file containing the observation wells.

1. Select the *Open* button .
2. In the *Open* dialog, change the *Files of type* selection to **Map Files (*.map)**.
3. Select the file named **obswells.map**.
4. Select the *Open* button.

You should see several observation points appear.

11.11.2 Transient Observation Data File

Now we will import the transient observation data associated with the observation wells. The transient observation data file format is almost identical to the pumping rate file format as follows:

name	date	time	head
"OBS_Q5"	12/3/1999	18:00:00	238.5
"OBS_Q5"	1/30/2000	7:38:25	834.7
"OBS_Q6"	3/27/2000	18:00:00	878.3
"OBS_Q6"	12/3/1999	18:00:00	733.2
"OBS_Q6"	12/5/1999	14:48:32	838.2
...			

The name column must be included. This tells GMS how to link the transient observation data to the points in the observation coverage.

The last column in the header line defines the name of the measurement. This measurement should be turned on in the *Coverage Setup* dialog before the first file is imported.

As each line is imported, the matching observation point is found and the observed head is added to the time series for the point.

This file should have the extension *.txt. The file is imported through the *Open* command in the *File* menu dialog.

To import the file:

1. Switch to the *Map* module .
2. Double-click on the **Observation Wells** coverage in the *Data Tree*.
3. In the column of *Obs. Points* attributes, turn on the *Trans. Head* attribute and click *OK*.
4. Select the *Open* button .
5. In the *Open* dialog, change the *Files of type* selection to **Text Files (*.txt)**.
6. Select the file named **trans_obs.txt**.
7. Select the *Open* button.
8. In the *File Import Wizard*, turn ON the *Heading row* option.
9. Under the *Set the column delimiters* section turn OFF the *Space* option. Click *Next*.
10. Set the *GMS data type* to **Transient observation data**.
11. In the *trans_head* column, set the *Type* to **Obs. Trans. Head**, and click *Finish*.

Now we have to re run MODFLOW.

1. Switch to the *3D grid* module .
2. Select the *Save* button .
3. Select the *MODFLOW | Run MODFLOW* command.
4. When MODFLOW finishes running, select *Close*.

The observation targets should now appear. Notice that if you change the time step in the *Data Tree*, the observation targets are updated accordingly.

11.11.3 Creating Transient Observation Plots

Finally, we will create two types of plots to view our transient observation data. The first plot is the *Error vs time step* plot. This plot displays the mean error (me), mean absolute error (mae), and the root mean squared error (rms) as a function of time.

1. Select the *Plot Wizard* button .

2. Change the plot type to *Error vs. Time Step*.
3. Select the *Next* button.
4. Select the *Finish* button to exit the dialog.

The plot shows that the error between the observed and computed values decreases slightly with time. The second type of plot that is useful for transient observation data is the time series plot.

1. Select the *Plot Wizard* button .
2. Change the plot type to *Time Series*.
3. Select the *Next* button.
4. Toggle on points **Point #8** and **Point #10**.
5. Turn on the *Calibration Target* toggle.
6. Select the *Finish* button to exit the dialog.

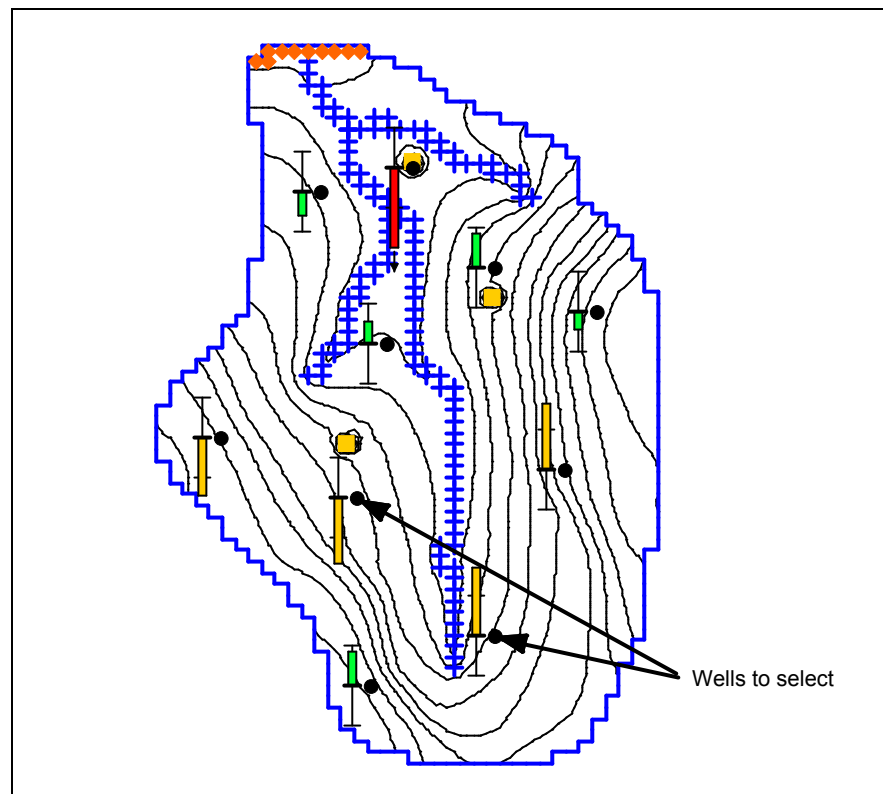


Figure 11-3 Observation Wells

Notice the dashed lines next to each curve. These dashed lines match the interval defined for each observation point. This makes it so you can easily see where the computed values fall within the observation target.

11.12 Conclusion

This concludes the *Managing Transient Data* tutorial. Here are the things that you should have learned in this tutorial:

- When you bring up the properties dialog for objects in the Map module, you can enter transient data by using the  button.
- You can import transient pumping data for wells and transient observation data. The wells or observation points must already exist.
- GMS can show dates and times as scalar values (0.0, 2.5 etc.) or in date/time format (12/03/2003).
- You must define your MODFLOW stress periods before you use the *Feature Objects | Map → MODFLOW / MODPATH* command.

Stochastic Modeling – Parameter Randomization

There is always a significant amount of uncertainty associated with a groundwater model. This uncertainty can be associated with the conceptual model or with the data and parameters associated with the various components of the model. Some model parameters such as hydraulic conductivity and recharge are particularly prone to uncertainty. Calibrating a model to a rich set of observation data (monitoring wells, stream flows, etc.) may reduce this uncertainty somewhat. However, calibration data are often scarce and even well-calibrated models have a high level of uncertainty.

One method for dealing with uncertainty is to utilize a stochastic modeling approach. With a non-stochastic approach, a single model is developed that represents the best estimate of the real system being simulated. This model is used to make predictions. With a stochastic approach, a set of models is constructed where each model in the set is thought to be equally probable. Each model is then used to make the prediction or simulate a given scenario and the results are used to estimate a probability or risk that a certain outcome will occur. While this approach still relies on underlying model assumptions to generate initial parameter estimates, it more honestly reflects the uncertainty associated with modeling.

GMS includes two basic methods for generating stochastic simulations: parameter randomization and indicator simulations. With the parameter randomization method, selected model parameters are randomized using either a Random Sampling or Latin Hypercube approach. Each combination of input parameters defines a model instance. With the indicator simulation approach,

multiple equally probable realizations of the aquifer heterogeneity are generated and each realization is used to define a model instance.

This tutorial illustrates how to develop a stochastic simulation using parameter randomization. Parameter randomization utilizes many of the tools described in the *Automated Parameter Estimation* tutorial. Therefore, we recommend that you complete that tutorial prior to beginning this one.

12.1 Description of Problem

The model we will be using in this tutorial is the same model featured in the *MODFLOW - Conceptual Model Approach* tutorial. This is a two layer model representing an aquifer in East Texas (see Figure 4-1). The model is bounded on the bottom and right sides by rivers represented with specified head boundaries and, on the north, by a no-flow boundary corresponding to a bedrock outcropping. The model includes two extraction wells and three drains. The model was developed to analyze the long-term consequences of a proposed landfill.

For this tutorial, we will randomize the recharge, the leakage from the landfill, and the hydraulic conductivity associated with the top layer. After developing multiple MODFLOW simulations using the Latin Hypercube sampling method, we will then simulate the contaminant transport resulting from each flow model using MT3DMS. Finally, we will process the results using the threshold analysis option in the *GMS Risk Analysis Wizard*.

12.2 Random Sampling vs. Latin Hypercube

GMS provides two methods for performing parameter randomization: Random Sampling and Latin Hypercube. With the Random Sampling method, the user specifies a mean, a standard deviation, a minimum value, and a maximum value for each parameter. In addition, the parameter can be specified as log transformed, which is typically the case for hydraulic conductivity. The user also specifies the number of simulations. For each simulation, a random number is generated for each parameter according to the specified distribution using the mean, standard deviation, maximum and minimum. GMS supports both normal and uniform distributions. The more simulations generated, the greater the confidence that all options have been explored.

The Latin Hypercube method is an attractive alternative to the Monte Carlo method since it allows for a greater degree of confidence with fewer model runs. This can be especially useful for complex models that require large amounts of computational time. As with the Random Sampling method, the user specifies the mean, standard deviation, minimum, and maximum for each parameter. For each parameter, the user also specifies a number of segments. The probability distribution curve for each parameter is then divided up into n

segments of equal probability. Figure 12-1 shows a normal distribution for a parameter that has six segments. Note that each segment has an equal area, not an equal distance between values.

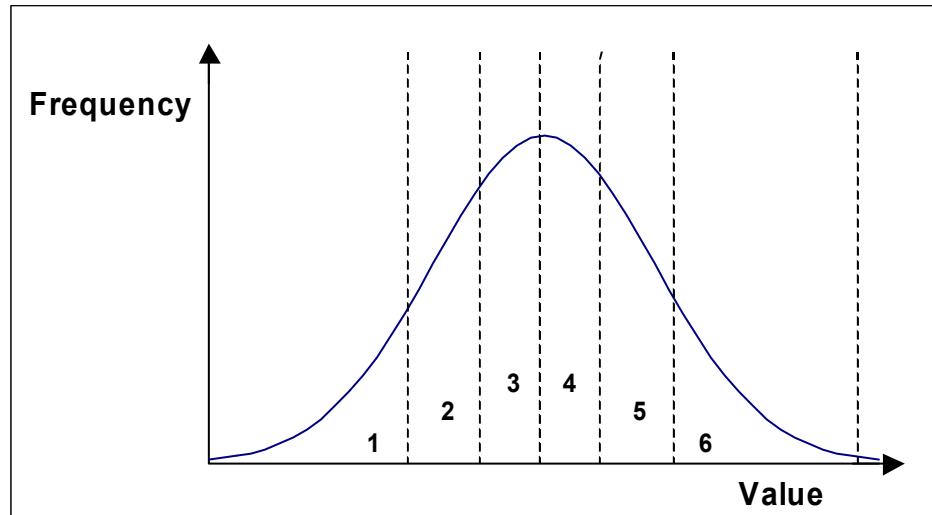


Figure 12-1 Latin Hypercube Segmentation for a Parameter with a Normal Distribution and Six Segments.

The idea behind the Latin Hypercube approach is that the parameter space (all possible combinations of parameter values) should be sampled as completely as possible with a limited number of model runs. Once the segments are defined, each parameter is then randomized until a value is found that lies within each probability segment. The random numbers for each parameter are combined with the random numbers from the other parameters such that all possible combinations of segments are sampled. The total number of model runs is the product of the number of segments for each parameter. For example, if you have three parameters with four segments each and one with five, the total number of simulations would be $4 \times 4 \times 4 \times 5 = 320$. In GMS, the total area under the probability curve is further limited by the specified maximum and minimum to give the maximum parameter range while still maintaining the best chance for model stability. The greater certainty from a smaller number of runs comes from guaranteeing that a more complete set of parameter combinations is tested. We will be using the Latin Hypercube approach in this tutorial.

12.3 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

12.4 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW
- Stochastic Modeling

You can see if these components are enabled by selecting the *File | Register* command.

12.5 Reading in the Project

First, we will read in a modeling project representing a completed MODFLOW model for the East Texas site:

1. Select the *Open* button .
2. Locate and open the **tutfiles\stochastic1** directory.
3. Select the file entitled **tex.gpr**.
4. Select the *Open* button.

You should see a MODFLOW model with a solution and a set of GIS coverages. The four coverages include a source/sink, a recharge, and two layer attribute coverages.

12.6 Model Parameterization

The first steps in setting up a stochastic model are similar to those used to start an inverse model – you need to “parameterize” the input. This involves identifying which parts of the model input we wish to randomize. The parameters with the highest uncertainty are obvious candidates for parameterization. When parameterizing a model, care should be taken to keep the number of selected parameters small. If too many parameters are chosen, unreasonably large numbers of model runs must be completed in order to adequately explore a sufficient combination of parameters. For this model, we will only use three parameters to ensure that the model run times will be fifteen minutes or less (depending on the speed of your computer).

12.7 Defining the Parameter Zones

The conceptual model approach used in GMS allows us to quickly define our parameter zones because the conceptual model consists of zones of recharge

and hydraulic conductivity defined by polygons. We will mark the polygons as parameter zones by assigning a “key value” to each polygon. The key value should be a value that is not expected to occur normally in the MODFLOW input. A negative value typically works well.

12.7.1 Setting up the Recharge Zones

First we will set up the recharge zones. The recharge polygons are shown in Figure 12-2. We will define a parameter for both the small polygon defining the landfill and the larger polygon encompassing the rest of the site. The key values associated with the two zones are shown on the polygons in the figure. The -200 zone represents recharge to the aquifer from rainfall. The -100 zone represents leakage from the landfill to the aquifer.

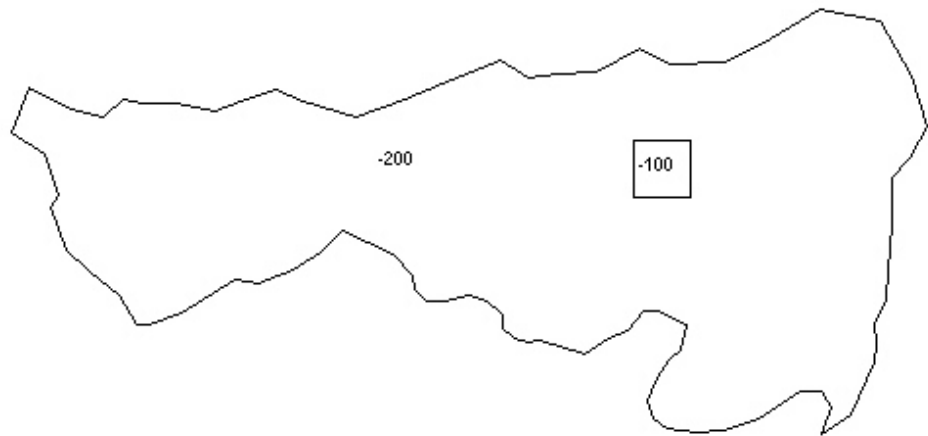


Figure 12-2 Recharge Zones Representing Aquifer Recharge (-200) and Landfill Leakage (-100).

To assign the key values to the polygons:

1. If necessary, switch to the *Map* module .
2. Expand the **East Texas** conceptual model by clicking on the plus symbol next to it in the *Data Tree*.
3. Switch to the *Recharge* coverage by selecting it from the *Data Tree*.
4. Select the *Select Polygon* tool .
5. Double click on each of the polygons show in Figure 12-2 and assign the appropriate key value to the *Recharge Rate* input field.

12.7.2 Setting up the Hydraulic Conductivity Zone

Next, we will parameterize the hydraulic conductivity for the top layer. For simplicity, we will assume that the hydraulic conductivity is constant for the entire layer.

1. Switch to the *Layer 1* coverage by selecting it from the *Data Tree*.
2. Double click on the polygon and assign a key value of **-300** to the *Horizontal K* input field.

12.7.3 Mapping the Key Values to the Grid Cells

Once the key values are assigned to the polygons, they must be mapped to the cells in the MODFLOW grid.

1. Select the *Feature Objects | Map → MODFLOW / MODPATH* command.
2. Select *OK* at the prompt.

12.8 Selecting the Stochastic Option

Before we edit the parameter data, we will turn on the *Stochastic* option. This option is located in the *Global Options* dialog.

1. Switch to the *3D Grid* module .
2. Select the *MODFLOW | Global Options* command.
3. In the *Run options* section of the dialog, select the *Stochastic Simulation* option.
4. Choose *OK* to exit the dialog.

12.9 Editing the Parameter Data

Two options are available when running a stochastic simulation using parameter zones – Random Sampling and Latin Hypercube. With Random Sampling, the total number of runs is specified directly in the *Parameters* dialog. With the Latin Hypercube method, the total number of MODFLOW runs is calculated from the number of segments specified for each parameter. We are going to use the Latin Hypercube method and we will use three parameters and give each parameter three segments for a total of 27 (3*3*3) MODFLOW runs.

Now we will create a list of parameters and enter a mean and standard deviation for each parameter that defines a normal probability distribution curve for the parameter value. We will also define bounds for the parameters to keep the values within an acceptable range.

1. Select the *MODFLOW | Parameters* command.

This dialog is used to manage the list of parameters and it is explained in detail in the *Automated Parameter Estimation* tutorial.

2. Select the *Initialize From Model* button.

Note that all three parameters were automatically found. Also note that the parameters have been given a default name. The next step is to enter a starting (mean), minimum, and maximum value for each parameter. You should notice that the usage fields have been set to *stochastic*. GMS will only perturb the parameters that are labeled as *stochastic* regardless of the values in the other fields.

3. Enter the following data into the parameters spreadsheet

Name	Mean Value	Min Value	Max Value
HK_300	16	1	100
RCH_200	0.0288	0.01	0.05
RCH_100	0.0003	0.0001	0.0005

4. For the hydraulic conductivity parameter, turn on the *Log transform* option.
5. Enter the following values for the standard deviation and number of segments:

Name	Std. Deviation	Num Segments
HK_300	0.5	3
RCH_200	0.01	3
RCH_100	0.001	3

6. Click on the *Repopulate Runs* button. Scroll down in the spread sheet and notice that the parameter values for each run are displayed.
7. Select *OK* to exit the dialog.

12.10 Saving the Project and Running MODFLOW

We are now ready to save the project and run MODFLOW in Stochastic mode.

1. Select the *File | Save As* command.

2. Enter **mfsto.gpr** for the filename.
3. Select the *Save* button.
4. Select the *MODFLOW | Run MODFLOW* command.

MODFLOW is now running in Stochastic mode. The spreadsheet at the top shows the set of parameter values associated with each model run. The first column indicated whether or not each model run has converged. Some combinations of parameter values result in unstable models. The lower window shows the text output from MODFLOW.

Note: If you have room on your screen, you may wish to resize the output window by dragging the handle in the lower right corner of the window.

12.11 Reading in and Viewing the MODFLOW Solutions

Once all the MODFLOW runs are completed, you can read in the solutions.

1. Make sure the *Read solution on exit* toggle is checked and select the *Close* button.

When the MODFLOW dialog closes, another dialog appears that lists each MODFLOW solution and whether it converged. You now have the option of choosing which of the solutions you want to read in, but all converged model solutions are checked by default.

2. Select *OK* to exit the dialog.

You should see a new folder named **mfsto (MODFLOW)(STO)** appear in the *Data Tree*. You can expand this folder to see the results of the stochastic simulation. Clicking on individual solutions within the folder updates the contours on the MODFLOW grid to reflect the solution results. You may wish to click on several of the solutions to view the variety in the range of answers. Some of the solutions may indicate flooded cells. This means that the computed water table elevation is above the ground surface. Note that once an individual solution folder is selected in the *Data Tree*, you can use the up and down arrows on your keyboard to cycle through the solutions.

12.12 MT3DMS

Now we will run an MT3DMS model using the results from each MODFLOW solution generated by the stochastic flow simulation. The MT3DMS model consists of one species, leachate from the landfill, entering the model from mass flux in the recharge and traveling toward the river and nearby well. We will assign a concentration to the recharge coming from the landfill polygon. Because the recharge for the landfill area in the MODFLOW model was varied

as a parameter, the mass flux (recharge rate X concentration) of contaminant leaving the landfill will vary for each model run. We will then read in the computed transport solutions and perform a probabilistic threshold concentration analysis.

12.13 Reading in the MT3DMS Project

First, we will read in the MT3DMS project:

1. Select the *File | Save* command. This will save the project in its current state, including the stochastic solutions.
2. Select the *Open* button .
3. Locate and open the **tutfiles\stochastic1** directory.
4. Change the *Files of type* to **Model Super Files**.
5. Select the file entitled **leachate.mts**.
6. Select the *Open* button.

12.14 MT3DMS Model

The MT3DMS model we have imported is a simple transport model with a concentration assigned to the recharge at the cells in the location of the landfill. The initial concentration for the entire model is set to zero. All of the other sources/sinks have a zero concentration. The simulation is set to run for 3000 days with output every 300 days. The leachate plume should migrate to the south and be captured by the well or the river or both.

12.15 Selecting the MODFLOW Stochastic Simulation

The MT3DMS model is already set up for us, but we still need to specify that we want to run MT3DMS in batch mode with our stochastic MODFLOW solution.

1. From the *MT3D | Run Options* command.
2. Select the *Batch run with selected MODFLOW solution set* option. We currently have only one MODFLOW solution set in GMS so *mfsto (MODFLOW)(STO)* should appear in the combo box below the selected radio button.
3. Select the *OK* button to exit the dialog.

12.16 Saving and Running MT3DMS in Stochastic Mode

We are now ready to save the project and run MT3DMS using the MODFLOW stochastic results.

1. Select the *File | Save As* command.

Note that we can specify different names for the MODFLOW and MT3DMS model files using the controls at the bottom of the dialog. However, in this case, we will use the default names.

1. Select the *Save* button.
2. Select *Yes* to overwrite the existing project.
3. Select the *MT3D | Run MT3D* command.

MT3DMS is now running in stochastic mode. The spreadsheet at the top shows each model, and as each model run is completed, the spreadsheet will update the status for the run as converged or not converged. It will take several minutes for all 27 model runs to be completed.

12.17 Reading in and Viewing the MT3DMS Solutions

Once all the MT3DMS runs are completed, you can read in the solutions as follows:

1. Make sure the *Read solution on exit* toggle is checked and select the *Close* button.

As was the case with the MODFLOW solution, when the MT3DMS dialog closes, another dialog appears that lists each MT3DMS solution and whether or not it converged.

1. Select *OK* to exit the dialog.

You should see a new folder name *mfssto (MT3DMS)(STO)* appear below the MODFLOW solutions in the *Data Tree* window. Once again, you can expand this folder and click on individual solutions to see the results of the stochastic transport simulation.

12.18 Threshold Analysis

Now that we have imported the MT3DMS solution set, we can perform a threshold analysis on the computed leachate concentrations. A threshold analysis can be used to generate a data set representing the probability that one or more user-defined threshold conditions is satisfied. For our case, we want to

generate a plot indicating the probability that the leachate concentration exceeds 10.0. To do this, we will set up a rule to mark leachate concentrations above 10.0. GMS then searches through all the selected solutions and for each cell it counts how many times the leachate concentration is exceeded. This number is then divided by the total number of solutions (27 in our case). These results are then contoured as a probability threshold dataset.

1. Select the MT3DMS solution set, *mfsto (MT3DMS)(STO)*, from the *Data Tree* window. This is the folder that contains the individual MT3DMS solutions.
2. While the MT3DMS solution set is selected in the window, right click the solution set and choose *Risk Analysis*. This brings up the *Risk Analysis Wizard*.
3. Verify that **MT3DMS** is selected in the list box, and select the *Next* button.

This next step in the *Risk Analysis Wizard* allows you to set up rules. Because we only have one contaminant, leachate, we only need one rule.

1. In the *Value* field for the first rule, enter a concentration of **10**.
2. Change the *Operator* to **>**.
3. Change the *Analysis title* to **above10**.
4. Choose the *Finish* button.

When the *Risk Analysis Wizard* finishes, a new data set, *above10*, will be added to the *mfsto (MT3DMS)(STO)* folder. This data set contains the probability that the leachate concentration will be above 10.0 for each of the time steps of our MT3DMS model. The best way to view this dataset is to turn on color filled contours.

1. Select the *Data | Contour Options* command.
2. Change the *Contour Method* to **Color Fill**.
3. Select the *Color Ramp* button to bring up the *Color Ramp Options* dialog.
4. Make sure the *Legend* box is checked.
5. Select *OK* on both dialogs to exit.

You should now see a probability plume extending from the landfill. You can cycle through the time steps in the *Time Step* window below the *Tree Window* to see the probabilities at the different times.

12.19 Conclusion

This concludes the *Stochastic Modeling – Parameter Randomization* tutorial. Here are the things that you should have learned in this tutorial:

- GMS supports two types of stochastic approaches: parameter randomization and indicator simulations
- With parameter randomization, you can do random sampling, latin hypercube sampling, or user defined sampling.
- You can run an MT3DMS model against all the stochastic MODFLOW solutions, but currently GMS does not support running MT3DMS stochastically itself (randomizing the MT3DMS parameters).
- You can run the *Risk Analysis Wizard* on any folder of solutions. One of the options in the *Risk Analysis Wizard* is a threshold analysis.

Stochastic Modeling – Indicator Simulations

GMS supports two methods for performing stochastic simulations: parameter randomization and indicator simulations. The previous tutorial illustrated the parameter randomization approach. The indicator simulation approach is described in this tutorial. With the indicator simulation approach, multiple equally probable “realizations” of the aquifer stratigraphy are generated. These realizations represent different distributions of material (indicator) zones within the aquifer. A set of aquifer properties is associated with the materials and the model is run once for each of the N realizations.

In GMS, the multiple realizations of the aquifer heterogeneity are typically generated using the T-PROGS software. T-PROGS can be used to generate two types of output: multiple material sets (arrays of material ids), or multiple MODFLOW HUF input sets. In each case, GMS can launch MODFLOW in batch mode and generate a flow solution for each model instance. For this tutorial we will be using a pre-defined set of material sets generated by T-PROGS. The steps involved in running a T-PROGS simulation are described in the *T-PROGS* tutorial.

13.1 Description of Problem

The model for this tutorial is based on the Longhorn Army Ammunition Production (LHAAP) site in Texas used in the *T-PROGS* tutorial. While we will be using the same site boundaries, the grid used in this simulation will have only one layer to facilitate a shorter run time. We will use a pre-defined T-PROGS simulation containing 30 material sets. The material sets will be

used with the stresses and boundary conditions depicted in Figure 13-1. There is a small drinking water well on the right side of the model. This well averages $25 \text{ ft}^3/\text{d}$. The regional ground water flow is from left to right. We will use specified head boundaries at the left and right edges of the model at 180 ft and 170 ft, respectively.

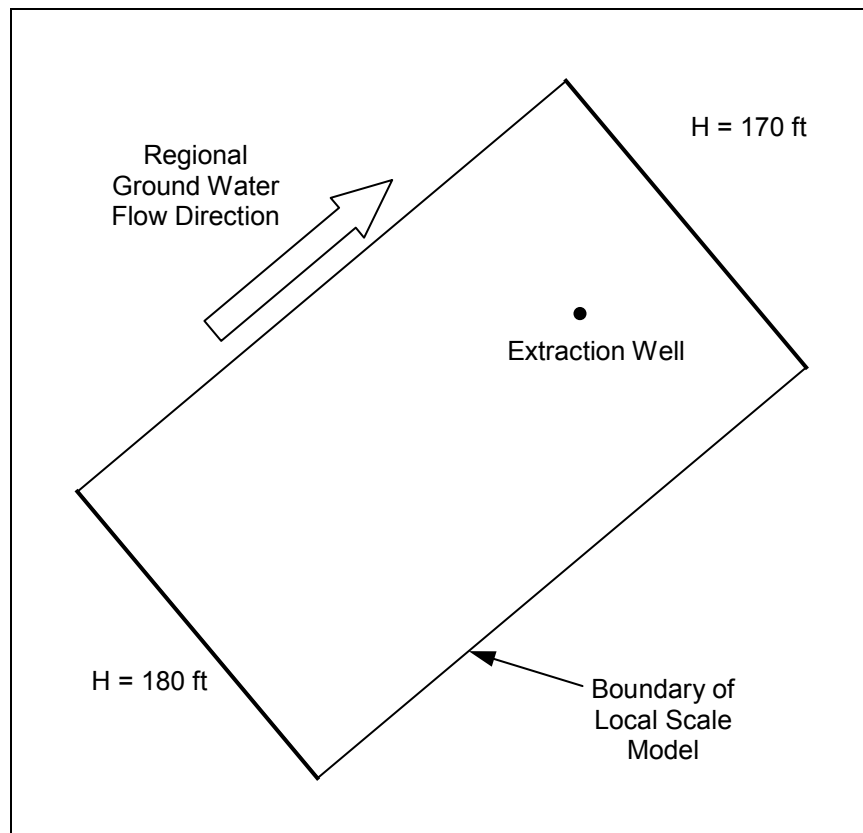


Figure 13-1 Conceptual Representation of Site to be Modeled.

Once the model is set up, we will run MODFLOW in stochastic mode to generate 30 solutions. We will then run the *Risk Analysis Wizard* to generate a data set representing probability of capture by the extraction well. We will contour this data set to illustrate capture zone boundaries for different probabilities of capture.

13.2 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *File | New* command to ensure the program settings are restored to the default state.

13.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW
- Stochastic Modeling

You can see if these components are enabled by selecting the *File | Register* command.

13.4 Reading in the Project

First, we will read in a project containing the MODFLOW model and the material sets generated by T-PROGS:

1. Select the *Open* button .
2. Locate and open the **tutfiles\stochastic2** directory.
3. Select the file entitled **lhaap.gpr**.
4. Select the *Open* button.

You should see a one layer MODFLOW model rotated at a 40 degree angle showing a four-material distribution. To view the material sets generated by T-PROGS:

1. Expand the *Material Sets* folder in the *Data Tree*.
2. Expand the *Simulation* folder.
3. Click on any of the material sets labeled **Simulation X**. You may wish to use the up and down arrow keys on your keyboard to cycle through the material sets.

13.5 The MODFLOW Model Data

Most of the MODFLOW data for our model (boundary conditions, well pumping rate, top and bottom elevations, etc.) has already been entered. However, we will review some of the MODFLOW data that are somewhat more unique to this type of simulation.

1. Select the *MODFLOW | LPF Package* command.

At the top of the dialog, notice that the *Use material ids* option is selected for the *Layer property entry method*. This means that we will not enter an array of K (hydraulic conductivity) values as is normally the case with MODFLOW. Rather, we will use material ids to define the K values.

2. Select the *Material IDs* button.

This dialog illustrates the material IDs assigned to cells. These material IDs are inherited from the active material set generated by T-PROGS.

3. Select the *OK* button to exit the *Material IDs* dialog.
4. Select the *Material Properties* button.

This dialog is used to assign aquifer properties, including hydraulic conductivity, to each of the materials used by the model. As you click on each of the materials in the list, you will notice that a value has been assigned for Kh and Kv for each material. Since this is a one layer model. Only the hydraulic conductivity value will be used. When the MODFLOW model is saved to disk, GMS uses the array of material IDs and the list of material properties to automatically generate the array of K values required by MODFLOW.

5. Select the *OK* button twice to exit both dialogs.

13.6 Selecting the Stochastic Option

Before running MODFLOW, we need to turn on the appropriate stochastic simulation options. First, we will select the stochastic run option:

1. Select the *MODFLOW | Global Options* command.
2. In the *Run Options* section of the dialog, select the *Stochastic Simulation* option.
3. Choose *OK* to exit the dialog.

Next, we need to specify that we will be using the material set method (as opposed to parameter randomization) in our stochastic simulation. When we choose the material set option, we must also specify which group (folder) of material sets we wish to use. In our case, we only have one group called *Simulation*.

1. Select the *MODFLOW | Stochastic* command.
2. Select the *Material sets* method.
3. Verify that **Simulation** shows up in the combo box below the *Material sets* option.

4. Choose *OK* to exit the dialog.

13.7 Saving the Project and Running MODFLOW

We are now ready to save the project and run MODFLOW in stochastic mode.

1. Select the *File | Save As* command.
2. Enter **matsto.gpr** for the filename.
3. Select the *Save* button.
4. Select the *MODFLOW | Run MODFLOW* command.

MODFLOW is now running in stochastic mode. As each model run finishes, the spreadsheet at the top will indicate whether or not the run converged.

13.8 Reading in and Viewing the MODFLOW Solutions

Once all the MODFLOW runs are completed, you can read in the solutions.

1. Make sure the *Read solution on exit* toggle is checked and select the *Close* button.
2. Select *OK* at the prompt to read in all converged solutions.

You should see a new folder named **matsto (MODFLOW)(STO)** appear in the *Data Tree*. You may wish to expand this folder and view the individual solutions. You will notice that the contours vary greatly depending on the distribution of materials. The head loss occurs primarily in the clay zones. As you view a particular solution, you may wish to select the material set in the *Data Tree* associated with that solution.

13.9 Displaying Pathlines

Before performing the probabilistic capture zone analysis, we will first view the capture zones corresponding to individual solutions.

1. Select the *MODPATH | Generate Particles at Wells* command.
2. Select the *OK* button to accept the default options.

You should see a set of pathlines appear. As you click on different MODFLOW solutions in the *Data Tree*, the pathlines will be automatically

updated. Notice how dramatically the capture zone changes from one solution to the next.

13.10 Probabilistic Capture Zone Analysis

Now that we have a MODFLOW stochastic solution set, we can perform a probabilistic capture zone analysis for the wells in our model. A probabilistic capture zone analysis is performed by placing one or more particles in each cell and tracking the particles forward in time using MODPATH to see if they reach a well. If any of the particles from a cell reach the well, a counter for the cell is updated. After running MODPATH on each of the MODFLOW solutions, the percentage of particles from a particular cell that are eventually captured by the well is computed and saved as the capture probability for the cell. The capture probability data set can then be contoured.

1. Select the MODFLOW solution set, *matsto (MODFLOW)(STO)*, from the *Data Tree* window.
2. While the MODFLOW solution set is selected in the window, right click on the solution set and choose *Risk Analysis*. This brings up the *Risk Analysis Wizard*.
3. Verify that **MODFLOW** is selected in the list box and select the *Probabilistic capture zone analysis* option.
4. Select the *Next* button.

You should now see the next page in the *Risk Analysis Wizard*. We can use this page to specify options for the position and number of particles for each cell. In the *Particle starting locations* area, we can choose to place particles on the water table or at the cell centers. We will use the default and place particles at the water table. We can also specify the tracking duration, although for this tutorial, we will be tracking the particles until they terminate (“To end”).

5. Select the *Finish* button.

At this point, the wizard should go away and a progress bar should appear at the bottom. When the computations are finished, a new data set, *well*, will be added to the *matsto (MODFLOW)(STO)* folder. This data set contains the probability that any particles placed at the water table will reach the well. The best way to view this data set is to turn on color filled contours.

6. Select the *Data | Contour Options* command.
7. Change the *Contour Method* to **Color Fill**.
8. Select the *Color Ramp* button to bring up the *Color Ramp Options* dialog.

9. Turn on the *Legend* option.

10. Select *OK* on both dialogs to exit.

You should now see a zone of probability extending from the well.

13.11 Conclusion

This concludes the Stochastic Modeling – Indicator Simulations tutorial. Here are the things that you should have learned in this tutorial:

- GMS supports two types of stochastic approaches: parameter randomization and indicator simulations
- The *Risk Analysis Wizard* can be used to do a probabilistic capture zone analysis.